

ARZ01-13456B

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I U C L I D

D a t a S e t

Existing Chemical ID: 64665-57-2
CAS No. 64665-57-2
EINECS Name sodium 4(or 5)-methyl-1H-benzotriazolide
EINECS No. 265-004-9
Molecular Weight 155
Molecular Formula C7H6N3.Na

Producer Related Part
Company:
Creation date: 15-JUL-1999

Substance Related Part
Company:
Creation date: 15-JUL-1999

Memo: SOCMA, Benzotriazoles Coalition

Printing date: 06-DEC-2001
Revision date:
Date of last Update: 06-DEC-2001

Number of Pages: 22

Chapter (profile): Chapter: 1, 2, 3, 4, 5, 7
Reliability (profile): Reliability: without reliability, 1, 2, 3, 4
Flags (profile): Flags: without flag, confidential, non confidential, WGK
(DE), TA-Luft (DE), Material Safety Dataset, Risk
Assessment, Directive 67/548/EEC, SIDS

1. General Information

1.0.1 OECD and Company Information

Type: lead organisation
Name: Synthetic Organic Chemicals Manufacturers Association (SOCMA),
Benzotriazoles Coalition
Street: 1850 M Street NW, Suite 700
Town: 20036 Washington, D.C.
Phone: 202-721-4100
Telefax: (202) 296-8120

05-DEC-2001

Type: cooperating company
Name: Bayer Corporation
Country: United States

05-DEC-2001

Type: cooperating company
Name: PMC Specialties Group, Inc.
Country: United States

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1.0.2 Location of Production Site

-

1.0.3 Identity of Recipients

-

1.1 General Substance Information

Substance type: organic
Physical status: liquid
05-DEC-2001

1.1.0 Details on Template

-

1.1.1 Spectra

-

1.2 Synonyms

CO-TT85
05-DEC-2001

1. General Information

Cobratec TT-50S
06-DEC-2001

Cobratec TT-85
05-DEC-2001

Preventol CI 7-50
05-DEC-2001

tolyltriazole, sodium salt
05-DEC-2001

1.3 Impurities

-

1.4 Additives

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1.5 Quantity

-

1.6.1 Labelling

-

1.6.2 Classification

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1.7 Use Pattern

-

1.7.1 Technology Production/Use

-

1.8 Occupational Exposure Limit Values

-

1.9 Source of Exposure

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1.10.1 Recommendations/Precautionary Measures

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1.10.2 Emergency Measures

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1. General Information

1.11 Packaging

-

1.12 Possib. of Rendering Subst. Harmless

-

1.13 Statements Concerning Waste

-

1.14.1 Water Pollution

-

1.14.2 Major Accident Hazards

-

1.14.3 Air Pollution

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1.15 Additional Remarks

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1.16 Last Literature Search

-

1.17 Reviews

-

1.18 Listings e.g. Chemical Inventories

-

2. Physico-chemical Data

2.1 Melting Point

Value: -5 - -10 degree C
Testsubstance: other TS: 50% aqueous solution of sodium tolyltriazole
05-DEC-2001 (1)

2.2 Boiling Point

Value: ca. 106 degree C at 1013 hPa
Decomposition: yes
Testsubstance: other TS: 50% aqueous solution of sodium tolyltriazole
05-DEC-2001 (1)

2.3 Density

Type: density
Value: 1.18 g/cm3 at 20 degree C
Testsubstance: other TS: 50% aqueous solution of sodium tolyltriazole
05-DEC-2001 (1)

2.3.1 Granulometry

-

2.4 Vapour Pressure

Value: .0000000000067 hPa at 25 degree C
Method: other (calculated): MPBPWIN (v1.31)
Year: 1999
GLP: no
Testsubstance: other TS: molecular structure
Result: Vapor Pressure Estimations (25 deg C):
(Using BP: 555.38 deg C (estimated))
(Using MP: 238.47 deg C (estimated))
VP: 8.02E-015 mm Hg (Antoine Method)
VP: 5.23E-012 mm Hg (Modified Grain Method)
VP: 1.74E-011 mm Hg (Mackay Method)
Selected VP: 5.23E-012 mm Hg (Modified Grain Method)
Reliability: (2) valid with restrictions
Accepted calculation method
Flag: Critical study for SIDS endpoint
06-DEC-2001 (2)

Value: .0533 hPa at 20 degree C
Testsubstance: other TS: 50% aqueous solution of sodium tolyltriazole
06-DEC-2001 (3)

Value: 25 hPa at 20 degree C
Testsubstance: other TS: 50% aqueous solution of sodium tolyltriazole
06-DEC-2001 (1)

2. Physico-chemical Data

2.9 Flammability

-

2.10 Explosive Properties

-

2.11 Oxidizing Properties

-

2.12 Additional Remarks

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3. Environmental Fate and Pathways

3.1.1 Photodegradation

Type: air
 INDIRECT PHOTOLYSIS
 Sensitizer: OH
 Conc. of sens.: 1560000 molecule/cm3
 Rate constant: .0000000000034188 cm3/(molecule * sec)
 Degradation: 50 % after 3.1 day
 Method: other (calculated): AOP Program (v1.89)
 Year: 1999 GLP: no
 Test substance: other TS: molecular structure
 Reliability: (2) valid with restrictions
 Accepted calculation method
 Flag: Critical study for SIDS endpoint
 06-DEC-2001

(2)

3.1.2 Stability in Water

Remark: Stable. Sodium Tolyltriazole dissolves in water, it does not hydrolyze. Sold as aqueous solution
 Flag: Critical study for SIDS endpoint
 06-DEC-2001

3.1.3 Stability in Soil

-

3.2 Monitoring Data (Environment)

-

3.3.1 Transport between Environmental Compartments

Type: fugacity model level III
 Media: other: air, water, soil, sediment
 Air (Level I):
 Water (Level I):
 Soil (Level I):
 Biota (L.II/III):
 Soil (L.II/III):
 Method: other: EPIWin Level III Fugacity Model
 Year: 1999

Result:	Media	Distribution (percent)	Half-Life (hr)	Emissions (kg/hr)	Fugacity (atm)
	Air	2.32e-006	75.1	1000	3.49e-020
	Water	43.5	360	1000	9.65e-022
	Soil	56.4	360	1000	4.03e-020
	Sediment	0.0754	1.44e+003	0	8e-022

	Media	Reaction (kg/hr)	Advection (kg/hr)	Reaction (percent)	Advection (percent)
	Air	0.000272	0.000295	9.08e-006	9.84e-006
	Water	1.07e+003	554	35.5	18.5
	Soil	1.38e+003	0	46	0
	Sediment	0.461	0.0192	0.0154	0.000639

Persistence Time: 424 hr

3. Environmental Fate and Pathways

Date: 06-DEC-2001

ID: 64665-57-2

Reaction Time: 520 hr
Advection Time: 2.3e+003 hr
Percent Reacted: 81.5
Percent Advected: 18.5
Reliability: (2) valid with restrictions
Flag: Critical study for SIDS endpoint
06-DEC-2001 (2)

3.3.2 Distribution

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3.4 Mode of Degradation in Actual Use

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3.5 Biodegradation

Type: aerobic
Inoculum:
Degradation: ca. 70 % after 28 day
Method: Directive 87/302/EEC, part C, p. 99 "Biodegradation:
Zahn-Wellens test"
Year: GLP: no data
Test substance: other TS: 50% aqueous solution of sodium tolyltriazole
06-DEC-2001 (1)

Type: aerobic
Inoculum:
Method:
Year: GLP:
Test substance:
Remark: See IUCLILD data set on methyl-1H-benzotriazole (CAS#
29385-43-1).
06-DEC-2001

3.6 BOD5, COD or BOD5/COD Ratio

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3.7 Bioaccumulation

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3.8 Additional Remarks

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AQUATIC ORGANISMS

4.1 Acute/Prolonged Toxicity to Fish

Type: static
 Species: Lepomis macrochirus (Fish, fresh water)
 Exposure period: 96 hour(s)
 Unit: Analytical monitoring:
 NOEC: 34
 LC50: > 173
 Method:
 Year: GLP: yes
 Test substance: other TS: 50% sodium tolyltriazole in water
 Method: Bluegill sunfish (initial bw = 5.0g) were acclimated for at least 5 days. During the experiment, the fish were not fed. On Day 0, 10 fish were introduced into test chambers containing nominal concentrations of 15, 23, 34, 51, 77, 115, and 173 ppm test substance. Fish were observed daily for mortality and signs of intoxication.
 Remark: Concentration in ppm
 Result: LC50 (96 hr) = > 173 ppm
 NOEC = 34 ppm

Conc	#fish	Mortality/ signs of intoxication				
		24	48	72	96	(hours)
Control	20	0/0	0/0	0/0	0/0	
15 ppm	10	0/0	0/0	0/0	0/0	
23 ppm	10	0/0	0/0	0/0	0/0	
34 ppm	10	0/0	0/0	0/0	0/0	
51 ppm	10	0/7	0/4	0/3	0/0	
77 ppm	10	1/9	1/9	1/9	1/9	
115 ppm	10	0/10	0/10	0/10	0/10	
173 ppm	10	0/10	0/10	0/10	0/10	

Clinical signs were present at Concentrations from 53 to 173. In general, the fish were either at the surface or on the bottom and exhibited almost total inactivity, but were hyperreactive to stimuli. Fish in the 51ppm group recovered by 96 hours, but none did in the higher concentrations. One fish died in the 77ppm group, which appears to be an unusual sensitivity since there were no deaths at the two higher concentrations.

Test condition: Water temperature and dissolved Oxygen measured daily; pH measured at beginning and end of study; hardness and alkalinity measured at beginning of study.

Photoperiod = 16 hours light/day
 Temperature: 15 - 18 degree C
 pH: 7.1 - 7.8
 Dissolved Oxygen: 5.4 - 8.4 mg/l
 Hardness: 143 - 147 mg/l
 Alkalinity: 54 - 55 mg/l
 Aeration: none

Reliability: (1) valid without restriction
 GLP study, Meets generally accepted scientific method and is

described in sufficient detail
 Flag: Critical study for SIDS endpoint
 06-DEC-2001 (5)

Type:
 Species: Salmo gairdneri (Fish, estuary, fresh water)
 Exposure period: 96 hour(s)
 Unit: mg/l Analytical monitoring:
 LC50: ca. 25
 Method:
 Year: GLP: yes
 Test substance: other TS: 50% sodium tolyltriazole in water
 Method: Rainbow trout (initial bw of 1.21 - 1.35g) were acclimated for at least 5 days. During the experiment, the fish were not fed and the water was not aerated. On Day 0, 10 fish were introduced into test chambers containing nominal concentrations of 16.6, 19.9, 23.2, 27.4, 32.5, 38.4, and 53.8 ppm test substance. Fish were observed daily for mortality and signs of intoxication. LC50 and 95% confidence limits were calculated according to Weil CS. 1952. Biometrics. 8:249.

Remark: Concentration in ppm
 Result: LC50 (24 hr) = > 53.8 ppm
 LC50 (48 hr) = 33 (31-35) ppm
 LC50 (72 hr) = 31 (29-32) ppm
 LC50 (96 hr) = 25 (24-26) ppm

Conc	#fish	Mortality/ signs of intoxication			
		24	48	72	96 (hours)
Control	20	0/0	0/0	0/0	0/0
16.6 ppm	10	0/0	0/0	0/0	0/0
19.9 ppm	10	0/0	0/1	0/4	0/4*
23.2 ppm	10	0/0	0/10	1/9*	1/9*
27.4 ppm	10	0/2	0/10*	0/10*	10/-*
32.5 ppm	10	0/10	9/1*	9/1*	9/1*
38.4 ppm	10	0/9	5/5*	9/1*	10/-
53.8 ppm	10	0/10	10/-*	10/-	10/-

* mortality values used to calculate the LC50.
 Test condition: Water temperature and dissolved Oxygen measured daily; pH measured at beginning and end of study; hardness and alkalinity measured at beginning of study.

Photoperiod = 16 hours light/day
 Temperature: 9.0 - 12.3 degree C
 pH: 7.1 - 8.6
 Dissolved Oxygen: 3.4 - 18.8 mg/l
 Hardness: 151 - 163 mg/l
 Alkalinity: 56 - 70 mg/l

Reliability: (1) valid without restriction
 GLP study, Meets generally accepted scientific method and is described in sufficient detail

Flag: Critical study for SIDS endpoint
 06-DEC-2001 (6)

4. Ecotoxicity

Date: 06-DEC-2001

ID: 64665-57-2

Type:
Species: Brachydanio rerio (Fish, fresh water)
Exposure period: 96 hour(s)
Unit: mg/l Analytical monitoring:
LC0: 100
LC50: 122
Method:
Year: GLP:
Test substance: other TS: 50% sodium tolyltriazole in water
06-DEC-2001 (1)

Type:
Species: Lepomis macrochirus (Fish, fresh water)
Exposure period: 96 hour(s)
Unit: mg/l Analytical monitoring:
LC50: 191.2
Method:
Year: GLP:
Test substance: other TS: 50% Sodium Tolyltriazole in water
06-DEC-2001 (4)

Type:
Species: Salmo gairdneri (Fish, estuary, fresh water)
Exposure period: 96 hour(s)
Unit: mg/l Analytical monitoring:
LC50: 23.7
Method:
Year: GLP:
Test substance: other TS: 50% Sodium Tolyltriazole in water
06-DEC-2001 (4)

Type: other: calculated
Species: other
Exposure period: 96 hour(s)
Unit: mg/l Analytical monitoring:
LC50: 137 - 179
Method: other: ECOSAR v0.99e
Year: 1999 GLP: no
Test substance: other TS: molecular structure
Remark: Chemical may not be soluble enough to measure this predicted effect.
Result: ECOSAR v0.99e Class(es) Found

Benzotriazoles

Predicted ECOSAR Class	Organism	Duration	End Pt	mg/L
=====	=====	=====	=====	=====
Neutral Organic SAR:	Fish	14-day	LC50	3060.916
(Baseline Toxicity)				
Benzotriazoles:	Fish [CLOGP]	96-hr	LC50	179.610
Benzotriazoles:	Fish [SRC]	96-hr	LC50	137.079
Benzotriazoles:	Fish [CLOGP]		ChV	51.989

Reliability: Benzotriazoles: Fish [SRC] ChV 12.658
 (2) valid with restrictions
 Flag: Critical study for SIDS endpoint
 06-DEC-2001 (2)

4.2 Acute Toxicity to Aquatic Invertebrates

Type: static
 Species: Daphnia magna (Crustacea)
 Exposure period: 48 hour(s)
 Unit: mg/l Analytical monitoring:
 NOEC: 100
 LC50 : 280
 Method: other: according to TSCA Public Law 94-469 (1976) and USEPA
 Registration of Pesticides guidelines Fed. Reg.
 07/10/78:29696-29741(1978)
 Year: 1978 GLP: yes
 Test substance: other TS: 50% aqueous solution of sodium tolyltriazole
 Result: LC50 (24 hr) = 440 mg/l (320-560)
 LC50 (48 hr) = 280 mg/l (180-560)
 NOEC = 100 mg/l

Conc	Mortality/ total # Daphnia	
	24	48 (hours)
Control	0/20	0/20
100 mg/l	0/20	0/20
180 mg/l	0/20	0/20
320 mg/l	0/20	14/20
560 mg/l	19/20	20/20
1000 mg/l	20/20	20/20

Clinical signs present at 180 mg/l were erratic behavior; at 320 mg/l Daphnia were either at the surface or on the bottom; and at 560 mg/l one exhibited loss of equilibrium.
 Test condition: Water temperature, pH, and dissolved Oxygen measured at beginning and end of study; hardness and alkalinity measured at beginning of study.

Photoperiod = 16 hours light/day
 Temperature: 20 degree C
 pH: 8.3 - 8.8
 Dissolved Oxygen: 7.4 - 8.1 mg/l
 Hardness: 225 - 275 ppm
 Alkalinity: 325 - 375 ppm
 Reliability: (1) valid without restriction
 GLP, National standards method
 Flag: Critical study for SIDS endpoint
 06-DEC-2001 (7)

4. Ecotoxicity

Date: 06-DEC-2001
ID: 64665-57-2

Type:
Species: Daphnia magna (Crustacea)
Exposure period: 48 hour(s)
Unit: mg/l Analytical monitoring:
LC50 : 245.7
Method:
Year: GLP:
Test substance:
06-DEC-2001 (4)

Type: other: calculated
Species: Daphnia sp. (Crustacea)
Exposure period: 48 hour(s)
Unit: mg/l Analytical monitoring: no
EC50: 596 - 1225
Method: other: ECOSAR v0.99e
Year: 1999 GLP: no
Test substance: other TS: molecular structure
Remark: Chemical may not be soluble enough to measure this predicted effect.
Result: ECOSAR v0.99e Class(es) Found

Benzotriazoles

Predicted				
ECOSAR Class	Organism	Duration	End Pt	mg/L
=====	=====	=====	=====	=====
Benzotriazoles:	Daphnid [CLOGP]	48-hr	LC50	1225.382
Benzotriazoles:	Daphnid [SRC]	48-hr	LC50	596.721
Benzotriazoles:	Daphnid [CLOGP]		ChV	30.333
Benzotriazoles:	Daphnid [SRC]		ChV	8.853
Reliability:	(2) valid with restrictions			
Flag:	Critical study for SIDS endpoint			
06-DEC-2001				(2)

4.3 Toxicity to Aquatic Plants e.g. Algae

Species: Selenastrum capricornutum (Algae)
 Endpoint: growth rate
 Exposure period: 96 hour(s)
 Unit: Analytical monitoring:
 NOEC: 10
 EC50: 26.2
 Method:
 Year: GLP: yes
 Test substance: other TS: 50% aqueous solution of sodium tolyltriazole
 Method: Selenastrum capricornutum (2×10^4 cells/ml) were exposed to test solutions of 0, 10, 30, 90, 270, and 810 mg/l (nominal concentrations) for four days and observed during a four day withdrawal period. Growth was monitored by cell counts and estimated biomass.

Comparison of cell numbers and biomass during exposure and withdrawal were made using Duncan's multiple range test with $\alpha = 0.05$. Dose-response analysis was done by probit method using log nominal concentrations. Biomass was estimated as: biomass (mg) = # cells x cell volume x 3.6×10^{-7} .

Remark: Concentration in ppm
 Result: Growth EC50 (96hr) = 26.2 ppm (16.6- 36.7)
 Biomass EC50 (96hr) = 32.0 ppm (4.1 - 78.7)
 NOEC = 100 ppm
 Lowest algastatic concentration = 270 ppm
 No level tested was algacidal.

Conc	cell counts		
	0	4	8 (days)
Control			
A	488	2211	26626
B	474	9017	60244
C	449	13473	58829
10 ppm			
A	584	4868	
B	551	8907	
C	602	3450	
30 ppm			
A	414	4809	63350
B	501	3850	54189
C	530	2620	51315
90 ppm			
A	454	2017	54920
B	551	1548	54570
C	501	3066	59239
270 ppm			
A	592	619	19552
B	483	180	23932
C	369	129	12171
810 ppm			
A	575	436	4071
B	609	291	2022

4. Ecotoxicity

Date: 06-DEC-2001

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Test condition: C 488 165 2008
The cultures were kept at 26-27 degree C with 400 +/-40 footcandles continuous cool-white fluorescent illumination and were continually oscillated on a platform at 100 rpm. Each concentration was tested in triplicate.

Reliability: (1) valid without restriction
GLP study, Meets generally accepted scientific method and is described in sufficient detail

Flag: Critical study for SIDS endpoint
06-DEC-2001 (8)

Species: other algae

Endpoint:

Exposure period: 96 hour(s)

Unit: mg/l Analytical monitoring: no

EC50: 50 - 56

Method: other: ECOSAR v0.99e

Year: 1999 GLP: no

Test substance: other TS: molecular structure

Result:

ECOSAR Class	Organism	Duration	End Pt	mg/L
=====	=====	=====	=====	=====
Benzotriazoles:	Green Algae [CLOGP]	96-hr	EC50	56.779
Benzotriazoles:	Green Algae [SRC]	96-hr	EC50	50.768
Benzotriazoles:	Algae [CLOGP]		ChV	12.608
Benzotriazoles:	Algae [SRC]		ChV	7.153

Reliability: (2) valid with restrictions

Flag: Critical study for SIDS endpoint
06-DEC-2001 (2)

4.4 Toxicity to Microorganisms e.g. Bacteria

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4. Ecotoxicity

4.5 Chronic Toxicity to Aquatic Organisms

4.5.1 Chronic Toxicity to Fish

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4.5.2 Chronic Toxicity to Aquatic Invertebrates

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TERRESTRIAL ORGANISMS

4.6.1 Toxicity to Soil Dwelling Organisms

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4.6.2 Toxicity to Terrestrial Plants

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4.6.3 Toxicity to other Non-Mamm. Terrestrial Species

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4.7 Biological Effects Monitoring

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4.8 Biotransformation and Kinetics

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4.9 Additional Remarks

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5. Toxicity

5.1 Acute Toxicity

5.1.1 Acute Oral Toxicity

Type: LD50
 Species: rat
 Strain: Wistar
 Sex: male/female
 Number of Animals: 10
 Vehicle:
 Value: ca. 1980 mg/kg bw
 Method:
 Year: 1983 GLP: no data
 Test substance: other TS: 50% sodium tolyltriazole in water
 Method: 5 rats/sex/dose, 5 doses: 1.0, 1.3, 1.6, 1.8, 2.5, 2.8 ml/kg bw, given by gavage, observation time: 14 d, pathologic examination of rats that died during observation time and of the survivors after termination.
 Remark: signs of intoxication: reduced general condition, prone position, rough fur, sedation.
 Pathologic examination:
 decedents: corrosion of the gastric mucous membranes;
 survivors: no findings.
 LD50: 1.66 ml/kg bw (ca. 1980 mg/kg bw)
 Reliability: (2) valid with restrictions
 Meets generally accepted scientific method and is described in sufficient detail.
 Flag: Critical study for SIDS endpoint
 06-DEC-2001 (9)

Type: LD50
 Species: rat
 Strain:
 Sex: male
 Number of Animals:
 Vehicle:
 Value: ca. 920 mg/kg bw
 Method:
 Year: GLP:
 Test substance: other TS: 50% sodium tolyltriazole in water
 06-DEC-2001 (4) (1)

5. Toxicity

Type: LD50
Species: rat
Strain:
Sex: female
Number of
Animals:
Vehicle:
Value: 640 - 735 mg/kg bw
Method:
Year: GLP:
Test substance: other TS: 50% sodium tolyltriazole in water
06-DEC-2001 (4) (1)

5.1.2 Acute Inhalation Toxicity

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5.1.3 Acute Dermal Toxicity

Type: LD50
Species: rabbit
Strain:
Sex:
Number of
Animals:
Vehicle:
Value: > 2000 mg/kg bw
Method:
Year: GLP:
Test substance: other TS: 50% sodium tolyltriazole in water
Remark: 24 hours of exposure; rabbits exhibited no symptoms
03-OCT-2000 (1)

5.1.4 Acute Toxicity, other Routes

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5.2 Corrosiveness and Irritation

5. Toxicity

5.2.1 Skin Irritation

Species: rabbit
Concentration: undiluted

Exposure: Semiocclusive
Exposure Time: 4 hour(s)
Number of Animals: 3
PDII:
Result: corrosive
EC classificat.:
Method: OECD Guide-line 404 "Acute Dermal Irritation/Corrosion"
Year: 1983 GLP: no data
Test substance: other TS: 50% aqueous solution of sodium tolyltriazole
Reliability: (1) valid without restriction
Guideline study

06-DEC-2001

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5.2.2 Eye Irritation

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5.3 Sensitization

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5.4 Repeated Dose Toxicity

Remark: Repeat dose studies (28 d or 18-24 month studies) conducted with tolyl triazole (29385-43-1) and 1H-Benzotriazole(95-14-7)

demonstrated an apparent reduction in toxicity with increasing molecular weight. The repeat dose toxicity of the sodium salt (CAS#64665-57-2) is expected to be similar to the repeat dose toxicity of tolyl triazole (29385-43-1) NOAEL = 150 mg/kg bw (oral- rat - 29 D) since the Sodium salt will dissociate to the methyl benzotriazole in aqueous solution.

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5.5 Genetic Toxicity 'in Vitro'

Remark: Mutagenicity testing has been conducted on tolyl triazole (29385-43-1) and 1H-Benzotriazole(95-14-7). The weight of evidence for the members of this category indicates these chemicals are not mutagenic or clastogenic. By bridging existing data to the sodium salt, which will dissociate to the methyl benzotriazole in aqueous solution, the mutagenicity aspect of the category has been evaluated adequately.

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5. Toxicity

5.6 Genetic Toxicity 'in Vivo'

Remark: Mouse micronucleus tests have been conducted on tolyl triazole (29385-43-1) and 1H-Benzotriazole(95-14-7). Both resulted in Negative results. There are also carcinogenicity studies on 1H-Benzotriazole(95-14-7). By bridging existing data to the sodium salt, which will dissociate to the methyl benzotriazole in aqueous solution, the mutagenicity aspect of the category has been evaluated adequately.

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5.7 Carcinogenicity

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5.8 Toxicity to Reproduction

Remark: The 78 week oral study of 1H-benzotriazole (95-14-7) in Fischer 344 rats and the 104 week oral study of 1H-benzotriazole in B6C3F1 mice did not find any evidence of pathology in the reproductive organs. The organs examined were: prostate/testis/epididymis of males and uterus/ovaries of females.

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(12)

5.9 Developmental Toxicity/Teratogenicity

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5.10 Other Relevant Information

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5.11 Experience with Human Exposure

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6. References

- (1) Safety Data Sheet Bayer AG, 09.02.1999
- (2) Meylan W. and Howard P. (1999) EPIWin Modeling Program. Syracuse Research Corporation. Environmental Science Center, 6225 Running Ridge Road, North Syracuse, NY 13212-2510.
- (3) PMC Specialties Group, Inc., MSDS 08/16/99
- (4) PMC Specialties Group, Inc., MSDS 01/29/97
- (5) Study No. 84-066-02. Mobay Chemical Corporation. August 3, 1984.
- (6) Study No. 84-066-01. Mobay Chemical Corporation. June 15, 1984.
- (7) Analytical Bio-Chemistry Laboratories, Inc. Report #32028. August 24, 1984.
- (8) Study No. 84-060-02. Mobay Chemical Corporation. August 2, 1984.
- (9) Bayer AG data, E. Löser: Untersuchungen zur akuten oralen Toxizität an männlichen und weiblichen Ratten, June 1983.
- (10) Bayer AG data, Suberg H., Prüfung auf primär reizende/ätzende Wirkung an der Kaninchenhaut, January, 1984
- (11) IUCLID data sets on CAS Nos. 95-14-7 and 29385-43-1
- (12) NTIS PB#285202 March, 1978. Bioassay of 1H-benzotriazole for possible carcinogenicity. CAS No. 95-14-7

7. Risk Assessment

7.1 End Point Summary

-

7.2 Hazard Summary

-

7.3 Risk Assessment

-

I U C L I D

D a t a S e t

Existing Chemical	ID: 95-14-7
CAS No.	95-14-7
EINECS Name	benzotriazole
EINECS No.	202-394-1
Molecular Weight	119.1
Molecular Formula	C6H5N3

Producer Related Part

Company:	
Creation date:	15-JUL-1999

Substance Related Part

Company:	
Creation date:	15-JUL-1999

Memo:	SOCMA, Benzotriazoles Coalition
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Printing date:	26-DEC-2001
Revision date:	
Date of last Update:	26-DEC-2001

Number of Pages:	35
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Chapter (profile):	Chapter: 1, 2, 3, 4, 5, 7
Reliability (profile):	Reliability: without reliability, 1, 2, 3, 4
Flags (profile):	Flags: without flag, confidential, non confidential, WGK (DE), TA-Luft (DE), Material Safety Dataset, Risk Assessment, Directive 67/548/EEC, SIDS

1. General Information

1.0.1 OECD and Company Information

Type: lead organisation
Name: Synthetic Organic Chemical Manufacturers Association,
Benzotriazoles Coalition
Street: 1850 M Street N.W., Suite 700
Town: 20036 Washington, D.C.
Country: United States
Phone: (202) 721-4100
Telefax: (202) 296-8120

03-DEC-2001

Type: cooperating company
Name: Bayer Corporation
Country: United States

03-DEC-2001

Type: cooperating company
Name: PMC Specialties Group, Inc.
Country: United States

03-DEC-2001

1.0.2 Location of Production Site

-

1.0.3 Identity of Recipients

-

1.1 General Substance Information

Substance type: organic
Physical status: solid
Purity: ca. 100 % w/w
04-DEC-2001

1.1.0 Details on Template

-

1.1.1 Spectra

-

1.2 Synonyms

1,2,3-BENZOTRIAZOLE
03-DEC-2001

1. General Information

BENZOTRIAZOLE

03-DEC-2001

Cobratec 99

Source: PMC Specialties Group

03-DEC-2001

Preventol CI 8-100

Source: Bayer Corporation

03-DEC-2001

1.3 Impurities

-

1.4 Additives

-

1.5 Quantity

-

1.6.1 Labelling

-

1.6.2 Classification

-

1.7 Use Pattern

-

1.7.1 Technology Production/Use

-

1.8 Occupational Exposure Limit Values

-

1.9 Source of Exposure

-

1.10.1 Recommendations/Precautionary Measures

-

1.10.2 Emergency Measures

-

1. General Information

1.11 Packaging

-

1.12 Possib. of Rendering Subst. Harmless

-

1.13 Statements Concerning Waste

-

1.14.1 Water Pollution

-

1.14.2 Major Accident Hazards

-

1.14.3 Air Pollution

-

1.15 Additional Remarks

-

1.16 Last Literature Search

-

1.17 Reviews

-

1.18 Listings e.g. Chemical Inventories

-

2. Physico-chemical Data

2.1 Melting Point

Value: 100 degree C
 Method: other: Handbook value
 GLP: no data
 Testsubstance: other TS: 1H-benzotriazole; purity not noted
 Reliability: (2) valid with restrictions
 Data from Handbook or collection of data
 Flag: Critical study for SIDS endpoint
 04-DEC-2001 (1)

Value: 94 - 99 degree C
 Testsubstance: other TS: 1H-benzotriazole; purity >99%
 Remark: stock point
 04-DEC-2001 (2) (3)

2.2 Boiling Point

Value: 204 degree C at 20 hPa
 Method: other: Handbook value
 GLP: no data
 Testsubstance: other TS: 1H-benzotriazole; purity not noted
 Reliability: (2) valid with restrictions
 Data from Handbook or collection of data
 Flag: Critical study for SIDS endpoint
 04-DEC-2001 (1)

Value: > 200 degree C
 Testsubstance: as prescribed by 1.1 - 1.4
 04-DEC-2001 (3)

Value: > 300 degree C
 Testsubstance: other TS: 1H-benzotriazole; purity >99%
 04-DEC-2001 (2)

2.3 Density

Type: density
 Value: ca. 1.19 g/cm3 at 100 degree C
 Testsubstance: as prescribed by 1.1 - 1.4
 Remark: mellifluousness
 Flag: Critical study for SIDS endpoint
 04-DEC-2001 (3)

Type: bulk density
 Value: ca. 500 kg/m3
 Testsubstance: as prescribed by 1.1 - 1.4
 04-DEC-2001 (3)

2.3.1 Granulometry

-

2. Physico-chemical Data

2.4 Vapour Pressure

Value: .000797 hPa at 25 degree C
 Method: other (calculated): MPBPWIN (v1.31)
 Year: 1999
 GLP: no
 Testsubstance: other TS: molecular structure
 Reliability: (2) valid with restrictions
 Accepted calculation method
 Flag: Critical study for SIDS endpoint
 04-DEC-2001 (4)

Value: ca. .00001 hPa at 25 degree C
 Testsubstance: as prescribed by 1.1 - 1.4
 04-DEC-2001 (3)

Value: .0533 hPa at 20 degree C
 Testsubstance: other TS: 1H-benzotriazole; purity >99%
 Flag: Critical study for SIDS endpoint
 04-DEC-2001 (2)

2.5 Partition Coefficient

log Pow: 1.34 at 22.7 degree C
 Method: other (measured)
 Year: 1991
 GLP: yes
 Testsubstance: as prescribed by 1.1 - 1.4
 Reliability: (1) valid without restriction
 GLP study
 Flag: Critical study for SIDS endpoint
 04-DEC-2001 (5)

log Pow: 1.167 at 25 degree C
 Method: other (calculated): KOWWIN Program (v1.65)
 Year: 1999
 GLP: no
 Testsubstance: other TS: molecular structure
 Result: Experimental Database Structure Match:
 Name : 1H-Benzotriazole
 CAS Num : 000095-14-7
 Exp Log P: 1.44
 Exp Ref : Hansch et al; 1995

Experimental Database Structure Match:
 Name : 2H-Benzotriazole
 CAS Num : 000273-02-9
 Exp Log P: 1.44
 Exp Ref : Sangster 1993

SMILES : c1ccc2nnnc2c1
 CHEM : 1H-Benzotriazole
 MOL FOR: C6 H5 N3
 MOL WT : 119.13

2. Physico-chemical Data

TYPE	NUM	LOGKOW	FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	6		Aromatic Carbon	0.2940	1.7640
Frag	3		Arom. Nitrogen [5-member ring]	-0.5262	-1.5786
Factor	1		1,2,3-Triazole correction	0.7525	0.7525
Const			Equation Constant		0.2290
				Log Kow	= 1.1669

Reliability: (2) valid with restrictions
 Accepted calculation method
 Flag: Critical study for SIDS endpoint
 04-DEC-2001 (4)

log Pow: 1.44
 Method: other (measured)
 Year:
 GLP: no data
 Testsubstance: other TS: 1H-Benzotriazole (CAS 95-14-7;) purity not noted
 09-MAY-2001 (6)

2.6.1 Water Solubility

Value: 1 - 5 mg/l at 23.7 degree C
 Method: other: no data
 GLP: no data
 Testsubstance: other TS: 1-H-benzotriazole; purity not noted
 Reliability: (2) valid with restrictions
 Data from Handbook or collection of data
 Flag: Critical study for SIDS endpoint
 04-DEC-2001 (7)

Value: ca. 19 g/l at 20 degree C
 Qualitative: miscible
 Testsubstance: other TS: 1H-benzotriazole; purity not noted
 Reliability: (2) valid with restrictions
 Data from Handbook or collection of data
 04-DEC-2001 (8) (3)

Qualitative: slightly soluble (0.1-100 mg/L)
 Method: other: Handbook value
 GLP: no data
 Testsubstance: other TS: 1H-benzotriazole; purity not noted
 Reliability: (2) valid with restrictions
 Data from Handbook or collection of data
 Flag: Critical study for SIDS endpoint
 04-DEC-2001 (1)

Value: 2 vol% at 20 degree C
 Testsubstance: other TS: 1H-benzotriazole; purity >99%
 04-DEC-2001 (2)

2. Physico-chemical Data

pKa: 8.2 at 25 degree C

Remark: The reaction suggests that benzotriazole will be less soluble in pH <7 (such as rainwater) and more soluble in solutions >7 (such as seawater) than in distilled water. Benzotriazole reacts with solutions of alkali metal hydroxides producing soluble alkali salts.

26-DEC-2001

(9)

2.6.2 Surface Tension

-

2.7 Flash Point

Value: ca. 195 degree C

Type:

Method: other: DIN 51584

Year:

Testsubstance: as prescribed by 1.1 - 1.4

04-DEC-2001

(3)

2.8 Auto Flammability

-

2.9 Flammability

Result:

Method: other: DIN 51794

Testsubstance: as prescribed by 1.1 - 1.4

Remark: ignition temperature: ca. 400 degrees C

04-DEC-2001

(3)

2.10 Explosive Properties

-

2.11 Oxidizing Properties

-

2.12 Additional Remarks

-

3.1.1 Photodegradation

Type: air

INDIRECT PHOTOLYSIS

Sensitizer: OH

Conc. of sens.: 1560000 molecule/cm3

Rate constant: .000000000001 cm3/(molecule * sec)

Degradation: 50 % after 10.7 day

Method: other (calculated): AOP Program (v1.89)

Year: 1999 GLP: no

Test substance: other TS: molecular structure

Result: AOP Program (v1.89) Results:

=====

SMILES : c1ccc2nnnc2c1

CHEM : 1H-Benzotriazole

MOL FOR: C6 H5 N3

MOL WT : 119.13

----- SUMMARY (AOP v1.89): HYDROXYL RADICALS -----

Hydrogen Abstraction = 0.0000 E-12 cm3/molecule-sec

Reaction with N, S and -OH = 0.0000 E-12 cm3/molecule-sec

Addition to Triple Bonds = 0.0000 E-12 cm3/molecule-sec

Addition to Olefinic Bonds = 0.0000 E-12 cm3/molecule-sec

Addition to Aromatic Rings = 0.0000 E-12 cm3/molecule-sec

**Addition to Fused Rings = 1.0000 E-12 cm3/molecule-sec

OVERALL OH Rate Constant = 1.0000 E-12 cm3/molecule-sec

HALF-LIFE = 10.696 Days (12-hr day; 1.5E6 OH/cm3)

Reliability: (2) valid with restrictions

Accepted calculation method

Flag: Critical study for SIDS endpoint

04-DEC-2001

(4)

3.1.2 Stability in Water

-

3.1.3 Stability in Soil

-

3.2 Monitoring Data (Environment)

-

3. Environmental Fate and Pathways

3.3.1 Transport between Environmental Compartments

Type: fugacity model level III
Media: other: air - water - sediment- soil
Air (Level I):
Water (Level I):
Soil (Level I):
Biota (L.II/III):
Soil (L.II/III):
Method: other: EPIWIN Level III Fugacity Model
Year: 1999
Result:

Media	Distribution (percent)	Half-Life (hr)	Emissions (kg/hr)	Fugacity (atm)
Air	4.6	257	1000	9.95e-011
Water	42.3	360	1000	5.94e-012
Soil	53.1	360	1000	1.45e-010
Sediment	0.0869	1.44e+003	0	4.8e-012

Media	Reaction (kg/hr)	Advection (kg/hr)	Reaction (percent)	Advection (percent)
Air	131	485	4.37	16.2
Water	859	446	28.6	14.9
Soil	1.08e+003	0	35.9	0
Sediment	0.442	0.0184	0.0147	0.000612

Persistence Time: 352 hr
Reaction Time: 510 hr
Advection Time: 1.13e+003 hr
Percent Reacted: 68.9
Percent Advected: 31.1

Reliability: (2) valid with restrictions
Accepted calculation method
Flag: Critical study for SIDS endpoint
04-DEC-2001

(4)

3.3.2 Distribution

-

3.4 Mode of Degradation in Actual Use

-

3. Environmental Fate and Pathways

3.5 Biodegradation

Type: aerobic
 Inoculum: activated sludge, industrial, non-adapted
 Concentration: 2 mg/l related to Test substance
 Degradation: 90 % after 28 day
 Testsubstance: 3 hour(s) 27 %
 7 day 55 %
 14 day 75 %
 21 day 83 %
 27 day 85 %
 Method: other: DIN 38 412 L 25 (Zahn-Wellens Test)
 Year: 1988 GLP: no
 Test substance: as prescribed by 1.1 - 1.4
 Remark: analytical monitoring of primary degradation
 Result: primary degradation with daylight: 90 % after 28 days
 degradation without daylight: 83 % after 28 days
 Reliability: (1) valid without restriction
 Meets National standards method (AFNOR/DIN)
 Flag: Critical study for SIDS endpoint
 04-DEC-2001 (10)

Type: aerobic
 Inoculum: predominantly domestic sewage, adapted
 Degradation: 0 % after 28 day
 Method: OECD Guide-line 301 D "Ready Biodegradability: Closed Bottle Test"
 Year: 1985 GLP: no
 Test substance: as prescribed by 1.1 - 1.4
 Remark: Test concentrations: 2.4, 8, 24, 80 mg/l
 Reliability: (1) valid without restriction
 Guideline study
 Flag: Critical study for SIDS endpoint
 04-DEC-2001 (11)

Type: aerobic
 Inoculum:
 Degradation: 0 % after 20 day
 Controlsubstance: Aniline
 Kinetic: 17 day 100 %
 Method: other: River Die-Away Test
 Year: GLP: no data
 Test substance: other TS: Cobratec 99; purity >99%
 04-DEC-2001 (12)

3.6 BOD5, COD or BOD5/COD Ratio

Remark: ThoD: 1948 mg/g
 COD: 1376 mg/g
 04-DEC-2001 (13)

3.7 Bioaccumulation

-

3.8 Additional Remarks

Remark: Elective cultures and continuous enrichment failed to demonstrate biodegradation of benzotriazole. Organisms were elected from soil samples from around Cardiff, activated sludge from a coke oven liquor treatment plant, microbially contaminated liquor wastes from a manufacturer of benzotriazole derivatives, microbially contaminated ship's engine cooling waters. No organisms that could be demonstrated to utilize benzotriazole for growth in solid or liquid minimal media were isolated from a small recirculating plant (TS conc. increased in the main tank (6 l, vigorously stirred and aerated, at ambient temp. 8 - 24 degrees C) from 0.5 to 3 mM in steps over 80 days of continuous operation and a proprietary anti-corrosion additive that contains benzotriazole). The minimum inhibitory conc. of the TS was estimated at 20 mM.

Source: Bayer AG Leverkusen

04-DEC-2001

(14)

AQUATIC ORGANISMS

4.1 Acute/Prolonged Toxicity to Fish

Type: static
Species: Brachydanio rerio (Fish, fresh water)
Exposure period: 96 hour(s)
Unit: mg/l Analytical monitoring: no
LC0: 100
LC50: > 100
Method: other: "Letale Wirkung beim Zebrabaerbling - Brachydanio rerio" (LC 0, LC 50, LC 100; 48-96 Stunden),
Verfahrensvorschlag Umweltbundesamt, Mai 1984
Year: 1984 GLP: no data
Test substance: as prescribed by 1.1 - 1.4
Result: time (hr) Abnormal swimming habit Mortality
24 3/10 0/10
48 10/10 0/10
72 10/10 0/10
96 10/10 0/10
Test condition: time (hr) temp (degree C) O2 (mg/l) pH
0 19.6 9.8 6.5
24 23.0 9.3 6.7
48 22.0 9.7 6.8
72 22.5 9.3 6.9
96 22.6 8.0 7.0
Reliability: (2) valid with restrictions
Meets generally accepted scientific standards, well documented
and acceptable for assessment
Flag: Critical study for SIDS endpoint
04-DEC-2001 (15)

Type:
Species: Salmo gairdneri (Fish, estuary, fresh water)
Exposure period: 96 hour(s)
Unit: mg/l Analytical monitoring: no data
LC50: 39
EC50 : 24.4
Method: other: Batelle Protocol
Year: GLP: no data
Test substance: other TS: Cobratec 99; purity >99%
Remark: LC50 generated by Binomial method; 95% confidence limits =
28.4- 49.5 mg/l
EC50 generated by Binomial method; 95% confidence limits =
21.0- 28.4 mg/l
Reliability: (2) valid with restrictions
Meets generally accepted scientific standards, well documented
and acceptable for assessment
Flag: Critical study for SIDS endpoint
04-DEC-2001 (12)

4. Ecotoxicity

Date: 26-DEC-2001

ID: 95-14-7

Type: flow through
Species: *Lebistes reticulatus* (Fish, fresh water)
Exposure period: 96 hour(s)
Unit: mg/l Analytical monitoring:
LC50: 28
Method:
Year: GLP: no data
Test substance: other TS: 1H-benzotriazole; purity not noted
Reliability: (2) valid with restrictions
04-DEC-2001 (16)

Type: flow through
Species: *Pimephales promelas* (Fish, fresh water)
Exposure period: 96 hour(s)
Unit: mg/l Analytical monitoring:
LC50: 28
Method:
Year: GLP: no data
Test substance: other TS: 1H-benzotriazole; purity not noted
Reliability: (2) valid with restrictions
04-DEC-2001 (16)

Type: flow through
Species: *Salmo gairdneri* (Fish, estuary, fresh water)
Exposure period: 96 hour(s)
Unit: mg/l Analytical monitoring:
LC50: 12
Method:
Year: GLP: no data
Test substance: other TS: 1H-benzotriazole; purity not noted
Remark: fingerlings
04-DEC-2001 (16)

Type: static
Species: *Lepomis macrochirus* (Fish, fresh water)
Exposure period: 96 hour(s)
Unit: mg/l Analytical monitoring:
LC50: 25
Method:
Year: GLP: no data
Test substance: other TS: 1H-benzotriazole; purity not noted
Reliability: (2) valid with restrictions
04-DEC-2001 (16)

Type: static
Species: *Pimephales promelas* (Fish, fresh water)
Exposure period: 96 hour(s)
Unit: mg/l Analytical monitoring:
LC50: 25
Method:
Year: GLP: no data
Test substance: other TS: 1H-benzotriazole; purity not noted
Reliability: (2) valid with restrictions
04-DEC-2001 (16)

4. Ecotoxicity

Date: 26-DEC-2001

ID: 95-14-7

Type: flow through
 Species: Lepomis macrochirus (Fish, fresh water)
 Exposure period: 96 hour(s)
 Unit: Analytical monitoring: no data
 TLm : 25
 Method:
 Year: GLP: no
 Test substance: other TS: Benzotriazole (BT-D); purity not noted
 Result: Median Tolerance Limit (TLm) = 27.5 ppm (48 hrs); 25.0 ppm (96 hrs)
 04-DEC-2001 (17)

Type: flow through
 Species: Pimephales promelas (Fish, fresh water)
 Exposure period: 96 hour(s)
 Unit: Analytical monitoring: no data
 TLm : 28
 Method:
 Year: GLP: no
 Test substance: other TS: Benzotriazole (BT-D); purity not noted
 Result: Median Tolerance Limit (TLm) = 30.2 ppm (48 hrs); 28.0 ppm (96 hrs)
 04-DEC-2001 (17)

Type: flow through
 Species: Salmo gairdneri (Fish, estuary, fresh water)
 Exposure period: 96 hour(s)
 Unit: Analytical monitoring: no data
 Tlm : 12
 Method:
 Year: GLP: no
 Test substance: other TS: Benzotriazole (BT-D); purity not noted
 Result: Median Tolerance Limit (TLm) = 15 ppm (48 hrs); 12 ppm (96 hrs)
 04-DEC-2001 (17)

Type: static
 Species: Lepomis macrochirus (Fish, fresh water)
 Exposure period: 96 hour(s)
 Unit: Analytical monitoring: no data
 TLm : 25
 Method: EPA OTS 797.1400
 Year: GLP: no
 Test substance: other TS: Benzotriazole (BT-D); purity not noted
 Result: Median Tolerance Limit (TLm) = 27.5 ppm (48 hrs); 25.0 ppm (96 hrs)
 04-DEC-2001 (17)

4. Ecotoxicity

Type: static
 Species: Pimephales promelas (Fish, fresh water)
 Exposure period: 96 hour(s)
 Unit: Analytical monitoring: no data
 TLm : 28
 Method:
 Year: GLP: no
 Test substance: other TS: Benzotriazole (BT-D); purity not noted
 Result: Median Tolerance Limit (TLm) = 30.2 ppm (48 hrs); 28.0 ppm (96 hrs)
 04-DEC-2001 (17)

4.2 Acute Toxicity to Aquatic Invertebrates

Type: static
 Species: Daphnia magna (Crustacea)
 Exposure period: 48 hour(s)
 Unit: mg/l Analytical monitoring: no
 EC0: 63
 EC50: 91
 EC100: 250
 Method: OECD Guide-line 202, part 1 "Daphnia sp., Acute Immobilisation Test"
 Year: 1991 GLP: yes
 Test substance: as prescribed by 1.1 - 1.4
 Result: Nominal Conc (mg/l) % immobilization

	24 hr	48 hr
0	0	0
63	0	0
88	25	60
125	40	90
177	40	95
250	50	100
354	100	
500	100	

Reliability: (1) valid without restriction
 GLP Guideline study
 Flag: Critical study for SIDS endpoint
 04-DEC-2001 (18)

4. Ecotoxicity

Type:
Species: Daphnia magna (Crustacea)
Exposure period: 48 hour(s)
Unit: mg/l Analytical monitoring: no data
LC50 : 141.6
Method: other: Battelle protocols
Year: GLP: no data
Test substance: other TS: Cobratec 99; purity >99%
Remark: LC50 generated by Probit method; 95% confidence limits =
127.7- 173.5 mg/l
Reliability: (2) valid with restrictions
Meets generally accepted scientific standards, well documented
and acceptable for assessment
Flag: Critical study for SIDS endpoint
04-DEC-2001 (12)

4.3 Toxicity to Aquatic Plants e.g. Algae

Species: Scenedesmus subspicatus (Algae)
Endpoint: growth rate
Exposure period: 72 hour(s)
Unit: mg/l Analytical monitoring: no
EC10: 58
EC50: 231
Method: other: DIN 38412 L 9
Year: 1992 GLP: yes
Test substance: as prescribed by 1.1 - 1.4
Result: Nominal Conc (mg/l) % inhibition (72 hr)

0	0
1	0
3.2	0
10	0
32	0
100	8.3
320	91.7
1000	100.0

Reliability: (1) valid without restriction
GLP Guideline study
Flag: Critical study for SIDS endpoint
04-DEC-2001 (19)

4. Ecotoxicity

Date: 26-DEC-2001

ID: 95-14-7

Species: Scenedesmus subspicatus (Algae)
Endpoint: biomass
Exposure period: 72 hour(s)
Unit: mg/l Analytical monitoring: no
EC10: 20
EC50: 102
Method: other: DIN 38412 L 9
Year: 1992 GLP: yes
Test substance: as prescribed by 1.1 - 1.4
Result: Nominal Conc (mg/l) % inhibition (72 hr)
0 0
1 2.7
3.2 2.0
10 0.7
32 10.7
100 47.6
320 96.3
1000 100.0
Reliability: (1) valid without restriction
GLP Guideline study
Flag: Critical study for SIDS endpoint
04-DEC-2001 (19)

Species: other aquatic plant: algae
Endpoint:
Exposure period: 96 hour(s)
Unit: mg/l Analytical monitoring: no data
NOEC: 4.1
LOEC: 8
EC50: 15.4
Method: other: Battelle protocol
Year: GLP: no data
Test substance: other TS: Cobratec 99; purity >99%
Remark: EC50 generated by Probit method; 95% confidence limits = 2.5-44.7 mg/l
NOEC and LOEC generated by ANOVA, Bonferroni test
04-DEC-2001 (12)

4.4 Toxicity to Microorganisms e.g. Bacteria

Type: aquatic
Species: activated sludge
Exposure period: 3 hour(s)
Unit: mg/l Analytical monitoring: no
EC50: 1060
EC95 : 3800
EC05 : 298
Method: ISO 8192 "Test for inhibition of oxygen consumption by activated sludge"
Year: 1991 GLP: yes
Test substance: as prescribed by 1.1 - 1.4
Remark: direct weight
Result: Nominal Conc (mg/l) % inhibition
180 0
320 8.3
560 15
1000 50
1800 75
Reliability: (1) valid without restriction
GLP Guideline study

04-DEC-2001

(20)

Type: other
Species: activated sludge of a predominantly domestic sewage
Exposure period: 5 day
Unit: mg/l Analytical monitoring:
EC0: 13.2
Method: other: Standard BOD test: Standard Methods for Examination of Water and Wastewater, 13th edition
Year: GLP:
Test substance: other TS: benzotriazole; purity not noted
Result: Concentrations of 0.66 to 13.2 mg/l benzotriazole did not affect the survival of the microbial seed during the 5 day test incubation at 20 degree C.

Sample Conc. (mg/l)	Colony count /ml
0 (initial)	54,570
0 (5 day)	151,000
0.66 (5 day)	207,000
3.3 (5 day)	217,000
6.6 (5 day)	183,000
13.2 (5 day)	164,000

Reliability: (1) valid without restriction
Guideline study

04-DEC-2001

(21)

4.5 Chronic Toxicity to Aquatic Organisms

4.5.1 Chronic Toxicity to Fish

-

4.5.2 Chronic Toxicity to Aquatic Invertebrates

Species: Daphnia magna (Crustacea)
Endpoint: other: immobilisation
Exposure period: 21 day
Unit: mg/l Analytical monitoring: yes
EC50: 76.9
NOEC : 25.9
Method: OECD Guide-line 202, part 2 "Daphnia sp., Reproduction Test"
Year: 1994 GLP: yes
Test substance: as prescribed by 1.1 - 1.4
Method: semi-static
analytical monitoring: TOC
To produce the stock solution, the test substance was weighed into water and treated for 1 hour in an ultrasonic device and, subsequently stirred for 1 hour with a magnetic stirrer.
Result: arithmetical mean of analytical values:
EC50: 76.9 mg/l (test substance) corresp. to 47.3 mg/l TOC
Reliability: (1) valid without restriction
GLP Guideline study
04-DEC-2001 (22)

Species: Daphnia magna (Crustacea)
Endpoint: reproduction rate
Exposure period: 21 day
Unit: mg/l Analytical monitoring: yes
NOEC: 25.9
LOEC: 76.9
EC50: 25.9 - 76.9
Method: OECD Guide-line 202, part 2 "Daphnia sp., Reproduction Test"
Year: 1993 GLP: yes
Test substance: as prescribed by 1.1 - 1.4
Remark: semi-static
analytical monitoring: TOC
To produce the stock solution the test substance was weighed into water and treated for 1 hour in an ultrasonic device and, subsequently stirred for 1 hour with a magnetic stirrer.
Result: arithmetical mean of analytical values:
EC50: 25.9 mg/l (test substance) corresp. to 15.3 mg/l TOC
76.9 mg/l (test substance) corresp. to 47.3 mg/l TOC
NOEC: 25.9 mg/l (test substance) corresp. to 15.3 mg/l TOC
LOEC: 76.9 mg/l (test substance) corresp. to 47.3 mg/l TOC
Reliability: (1) valid without restriction
GLP Guideline study
04-DEC-2001 (22)

4. Ecotoxicity

TERRESTRIAL ORGANISMS

4.6.1 Toxicity to Soil Dwelling Organisms

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4.6.2 Toxicity to Terrestrial Plants

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4.6.3 Toxicity to other Non-Mamm. Terrestrial Species

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4.7 Biological Effects Monitoring

-

4.8 Biotransformation and Kinetics

-

4.9 Additional Remarks

-

5. Toxicity

5.1 Acute Toxicity

5.1.1 Acute Oral Toxicity

Type: LD50
 Species: rat
 Strain: no data
 Sex: male/female
 Number of Animals: 10
 Vehicle: no data
 Value: 560 mg/kg bw
 Method: other
 Year: GLP: no data
 Test substance: other TS: Cobratec #99 (benzotriazole); purity >99%
 Method: 5 rats/sex/dose, single application of 4 dose levels, post exposure observation time: 14 d
 Remark: 398 mg/kg; mortality: 0/10; 502 mg/kg, mortality: 4/10; 632 mg/kg bw, mortality: 7/10; 795 mg/kg, mortality: 10/10
 Reliability: (2) valid with restrictions
 Meets generally accepted scientific standards, well documented and acceptable for assessment
 Flag: Critical study for SIDS endpoint
 04-DEC-2001 (23)

Type: LD50
 Species: rat
 Strain: other: Greenacres strain
 Sex: male
 Number of Animals: 5
 Vehicle: other: corn oil
 Value: 909 mg/kg bw
 Method: other
 Year: GLP: no data
 Test substance: other TS: benzotriazole; purity not noted
 Method: The test substance was administered by stomach tube to six groups of 5 male albino rats (weight range 305 - 370 g). The sample was administered in corn oil as a 10% or 50% wt/vol suspension. (Dosage levels of 46.4, 100, 215 mg/kg as 10 % wt/vol; 1000, 150 mg/kg as 50% wt/vol)

Food was withheld for 18 hrs prior to dosing, following which food and water was supplied ad libitum. All animals observed several times during day of dosing for gross signs of systemic toxicity and mortality and daily thereafter for 14 days. Gross autopsies were done on all animals. Statistical analysis of mortality data was done by "moving average" method (Weil, CS. Biometrics. 8:249. 1952)

Result: LD 50 = 909 mg/kg bw (95% conf. limit = 546 - 1510 mg/kg)

Time of death	Dose (mg/kg)					
	46.4	100	215	464	1000	2150
1 hr	0/5	0/5	0/5	0/5	0/5	1/5
2 hr	0/5	0/5	0/5	0/5	1/5	2/5

5. Toxicity

Date: 26-DEC-2001

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	4 hr	0/5	0/5	0/5	0/5	3/5	2/5
	24 hr	0/5	0/5	0/5	0/5	4/5	4/5
	2 days	0/5	0/5	0/5	0/5	4/5	4/5
	3 days	0/5	0/5	0/5	0/5	4/5	4/5
	4 days	0/5	0/5	0/5	0/5	4/5	4/5
	5 days	0/5	0/5	0/5	0/5	4/5	4/5
	6 days	0/5	0/5	0/5	0/5	4/5	4/5
	7-14 days	0/5	0/5	0/5	0/5	4/5	4/5

Reliability: (2) valid with restrictions
Meets generally accepted scientific standards, well documented
and acceptable for assessment

Flag: Critical study for SIDS endpoint

04-DEC-2001 (24)

Type: LD50
Species: rat
Strain: Sprague-Dawley
Sex: male/female
Number of
Animals: 10
Vehicle:
Value: 720 mg/kg bw
Method: other
Year: GLP: no data
Test substance: other TS: benzotriazole residue (sample 81469-B); purity not
noted
Method: Five male and five female rats/group were given a single oral
dose via blunt tipped canula. Doses levels were 316, 632,
892, 1260 mg/kg. Animals were observed for toxicity and
mortality for 14 days. All rats were subjected to a
macroscopic examination of the viscera at necropsy.
Remark: The LD50 value was calculated according to Litchfield and
Wilcoxon, 1949.
Reliability: (2) valid with restrictions
Meets generally accepted scientific standards, well documented
and acceptable for assessment

04-DEC-2001 (25)

5.1.2 Acute Inhalation Toxicity

Type: LC50
Species: rat
Strain: Sprague-Dawley
Sex: male/female
Number of
Animals: 10
Vehicle: other: as a dust
Exposure time: 4 hour(s)
Value: > 1.5 mg/l
Method: other
Year: GLP: no data
Test substance: other TS: benzotriazole; purity not noted
Method: The exposure was conducted for 4 hours at a target level of
2.5 mg/l. Exposure levels were determined by gravimetric

analysis during each hour of exposure. Particle size of the aerosiolized dust was determined using a cascade impactor.

BT was administered via inhalation as a dust, by whole body exposure. Physical observations for abnormal signs were conducted on all animals as a group at 15 minute intervals during the first hour of exposure, and hourly for the remainder of the exposure. All animals received detailed physical observations prior to exposure and upon removal from the chamber, hourly for two hours post exposure, and daily for the 14 day post-exposure period. All animals were sacrificed and complete postmortem examinations were performed.

Result: All animals survived the exposure and the 14-day post-exposure observation period. Signs of treatment included slight labored breathing and/or nasal discharge during the exposure or the first week following exposure. These symptoms abated during the second post-exposure week. Slight decreases in weight were observed on the day after exposure with a recovery thereafter. Postmortem examinations were unremarkable.

The mean gravimetric exposure concentration for the 4-hour exposure was determined to be 1.5 mg/l (considered to be the maximum attainable concentration).

**1.5 mg/l for 4 hours is considered equivalent to 6.0 mg/l for 1 hour

Reliability: (2) valid with restrictions
Meets generally accepted scientific standards, well documented and acceptable for assessment

Flag: Critical study for SIDS endpoint

04-DEC-2001

(26)

Type: LC50

Species: rat

Strain:

Sex: male

Number of
Animals: 10

Vehicle:

Exposure time: 3 hour(s)

Value: 1.91 mg/l

Method: other

Year: GLP: no data

Test substance: other TS: benzotriazole; purity not noted

Method: Five groups of ten male albino rats were exposed for 3 hours to different concentrations of benzotriazole as a fine aerosol.

Result: The LC50 was determined to be 1.91 mg/l (95% conf. limits = 1.59 - 2.29 mg/l)

Animals which survived the exposure were generally in very good health one-two days post exposure. The primary effect appeared to be pulmonary irritation which resulted intra-tracheal edema and a hemorrhagic type response in the lungs.

Reliability: (2) valid with restrictions

Meets generally accepted scientific standards, well documented
and acceptable for assessment

04-DEC-2001 (27)

5.1.3 Acute Dermal Toxicity

Type: LD50
Species: rabbit
Strain:
Sex: male/female
Number of Animals: 4
Vehicle: physiol. saline
Value: > 10000 mg/kg bw

Method: EPA OTS 798.1100
Year: GLP: no data
Test substance: other TS: BT-D (benzotriazole) sample no. SD-7413; purity not noted

Method: Dosage levels of 1000, 2150, 4640, 10000 mg/kg bw were applied to intact (2 animals/group) or abraded (2 animals/group) of male and female albino rabbits and occluded for 24 hours. Animals were observed for 14 days post exposure.

Result: No mortalities occurred at any dosage level. With the exception of purulent nasal discharge noted in occasional rabbits, all animals generally exhibited normal appearance and behavior throughout the study.

Reliability: (2) valid with restrictions
Guideline study

Flag: Critical study for SIDS endpoint

04-DEC-2001 (28)

Type: LD50
Species: rat
Strain: no data
Sex: male/female
Number of Animals:
Vehicle: no data
Value: > 2000 mg/kg bw

Method:
Year: 1984 GLP: no data
Test substance: other TS: benzotriazole; purity not noted

Method: other: acute dermal application and a 14 day post-treatment observation period (no further information)

Remark: Symptoms: Dyspnea, exophthalmus, ruffled fur and abnormal body position are symptoms commonly seen during observation time following administration of substances by gavage. No other symptoms which could be related to the treatment, especially no cutaneous changes, were observed.

24-MAY-2001 (29)

5. Toxicity

Type: LD50
Species: rabbit
Strain:
Sex:
Number of
Animals: 10
Vehicle:
Value: > 2000 ml/kg bw
Method: other
Year: GLP:
Test substance: other TS: Cobratec 99 (BT) Sample no. 6023; purity >99%
Method: Cobratec 99 was tested for Acute Dermal Toxicity in 10 rabbits
at 2000 mg/kg
Result: According to the code of Federal Regulations, the substance is
not toxic.
04-DEC-2001 (30)

5.1.4 Acute Toxicity, other Routes

Type: LD50
Species: mouse
Strain:
Sex:
Number of
Animals:
Vehicle:
Route of admin.: i.p.
Value: 1000 mg/kg bw
Method:
Year: GLP: no data
Test substance:
02-OCT-2000 (7)

Type: LD50
Species: mouse
Strain:
Sex:
Number of
Animals:
Vehicle:
Route of admin.: i.v.
Value: 238 mg/kg bw
Method:
Year: GLP: no data
Test substance:
02-OCT-2000 (7)

5. Toxicity

5.2 Corrosiveness and Irritation

5.2.1 Skin Irritation

Species: rabbit

Concentration:

Exposure:

Exposure Time:

Number of

Animals:

PDII:

Result: not irritating

EC classificat.:

Method:

Year:

GLP:

Test substance: as prescribed by 1.1 - 1.4

Remark: Exposure period: 4 hour

04-DEC-2001

(13)

5.2.2 Eye Irritation

Species: rabbit

Concentration: undiluted

Dose: 100 other: mg

Exposure Time: 72 hour(s)

Comment: not rinsed

Number of

Animals:

Result: highly irritating

EC classificat.:

Method: Draize Test

Year:

GLP: no data

Test substance: other TS: BT-D (benzotriazole) sample no. SD-7413 (Sherwin Williams Co.); purity not noted

Result: Irritative effects included moderate or marked conjunctivitis and corneal opacity, mild iritis, and conjunctival blanching in each rabbit. These signs remained relatively unchanged throughout the 72 hour observation period.

04-DEC-2001

(28) (2)

Species: rabbit

Concentration:

Dose:

Exposure Time:

Comment:

Number of

Animals:

Result: slightly irritating

EC classificat.:

Method:

Year:

GLP:

Test substance: as prescribed by 1.1 - 1.4

04-DEC-2001

(13)

5.3 Sensitization

Type: Guinea pig maximization test
Species: guinea pig
Number of Animals:
Vehicle:
Result: not sensitizing
Classification:
Method: OECD Guide-line 406 "Skin Sensitization"
Year: GLP: no data
Test substance: as prescribed by 1.1 - 1.4
Reliability: (1) valid without restriction
Guideline study

04-DEC-2001

(13)

5.4 Repeated Dose Toxicity

Species: rat Sex: male/female
Strain: Fischer 344
Route of admin.: oral feed
Exposure period: 78 weeks
Frequency of treatment: daily
Post. obs. period: 26-27 weeks
Doses: 6,700 and 12,100 ppm
Control Group: yes, concurrent no treatment
Method: other: EPA OTS 798.3300
Year: GLP: no data
Test substance: other TS: 1H-benzotriazole; purity > 99%
Method: Groups of 50 Fisher 344 rats of each sex were administered 1H-benzotriazole at one of two time-weighted average doses, either 6,700 or 12,100 ppm for 78 weeks. Except for five control and five high-dose rats of each sex, which were killed at week 78, all animals surviving at that time were observed for an additional 26-27 weeks. Controls consisted of groups of 50 untreated rats of each sex and were observed for 105-106 weeks. All rats surviving to week 104-106 were sacrificed and examined for tumors.
Remark: no clinical symptoms; no influence on mortality
Reliability: (1) valid without restriction
Meets generally accepted scientific standards, well documented and acceptable for assessment
Flag: Critical study for SIDS endpoint

26-DEC-2001

(31)

5. Toxicity

Date: 26-DEC-2001

ID: 95-14-7

Species: mouse Sex: male/female
Strain: B6C3F1
Route of admin.: oral feed
Exposure period: 104 weeks
Frequency of treatment: daily
Post. obs. period: 2 weeks
Doses: 11,700 and 23,500 ppm
Control Group: yes, concurrent no treatment
Method: other: EPA OTS 798.3300
Year: GLP: no data
Test substance: other TS: 1H-benzotriazole; purity > 99%
Method: Groups of 50 B6C3F1 mice of each sex were administered 1H-benzotriazole at one of two time-weighted average doses, either 11,700 or 23,500 ppm for 104 weeks, then observed for an additional 2 weeks. Controls consisted of groups of 50 untreated mice of each sex and were observed for 109 weeks. All mice surviving to week 106-109 were sacrificed and examined for tumors.
Remark: no clinical symptoms; no influence on mortality
Reliability: (1) valid without restriction
Meets generally accepted scientific standards, well documented and acceptable for assessment
Flag: Critical study for SIDS endpoint
26-DEC-2001 (31)

5.5 Genetic Toxicity 'in Vitro'

Type: HGPRT assay
System of testing: CHO cells
Concentration: without: 150, 300, 400, 500, 600, 800, 1000 µg/ml; with: 50, 100, 200, 350, 500, 700, 1000 µg/ml
Cytotoxic Conc.: without: 1000 µg/ml rel. survival: 82.4 % with: 500 µg/ml_ 19.1 %, 1000 µg/ml: 0.0 %
Metabolic activation: with and without
Result: negative
Method: OECD Guide-line 476 "Genetic Toxicology: In vitro Mammalian Cell Gene Mutation Tests"
Year: 1987 GLP: yes
Test substance: as prescribed by 1.1 - 1.4
Reliability: (1) valid without restriction
GLP Guideline study
Flag: Critical study for SIDS endpoint
04-DEC-2001 (32)

5. Toxicity

Type: Ames test
 System of testing: Salmonella typhimurium
 Concentration:
 Cytotoxic Conc.: no data
 Metabolic activation: no data
 Result: positive
 Method:
 Year: GLP: no data
 Test substance:
 04-DEC-2001 (33) (34)

5.6 Genetic Toxicity 'in Vivo'

Type: Micronucleus assay
 Species: mouse Sex:
 Strain: NMRI
 Route of admin.: gavage
 Exposure period: once
 Doses: 0, 800 mg/kg bw
 Result: negative
 Method: OECD Guide-line 474 "Genetic Toxicology: Micronucleus Test"
 Year: 1988 GLP: yes
 Test substance: as prescribed by 1.1 - 1.4
 Reliability: (1) valid without restriction
 GLP Guideline study
 Flag: Critical study for SIDS endpoint
 04-DEC-2001 (35)

5.7 Carcinogenicity

Species: rat Sex: male/female
 Strain: Fischer 344
 Route of admin.: oral feed
 Exposure period: 78 weeks
 Frequency of treatment: continuous
 Post. obs. period: 26-27 weeks
 Doses: 0, 6700, 12100 ppm
 Result: negative
 Control Group: yes, concurrent no treatment
 Method: EPA OTS 798.3300
 Year: GLP: no data
 Test substance: other TS: 1H-benzotriazole; purity > 99%
 Remark: In male rats, neoplastic nodules of the liver occurred at a statistically significant incidence in the high-dose group but the incidence in historic laboratory controls varies from 0-11%; therefore these tumors cannot clearly be associated with test sample administration.
 In female rats, incidence of endometrial stromal polyps was significant in the low-dose group, but not significant in the

5. Toxicity

Date: 26-DEC-2001

ID: 95-14-7

high-dose group; therefore cannot clearly be associated with
test sample administration.

Reliability: (1) valid without restriction
GLP Guideline study

26-DEC-2001 (31)

Species: mouse Sex: male/female
Strain: B6C3F1
Route of admin.: oral feed
Exposure period: 104 weeks
Frequency of
treatment: continuous
Post. obs.
period: 106 weeks
Doses: 0, 11700, 23500 ppm
Result: negative
Control Group: yes, concurrent no treatment
Method: EPA OTS 798.3300
Year: GLP: no data
Test substance: other TS: 1H-benzotriazole; purity > 99%
Remark: In female mice, incidence of alveolar/bronchiolar carcinomas
was statistically significant in the low-dose group, but not
significant in the high-dose group; therefore occurrence of
this tumor cannot clearly be associated with test sample
administration.

Reliability: (1) valid without restriction
GLP Guideline study

26-DEC-2001 (31)

Species: Sex:
Strain:
Route of admin.:
Exposure period:
Frequency of
treatment:
Post. obs.
period:
Doses:
Result:
Control Group:
Method: other: In vitro-Test
Year: GLP:
Test substance:
Remark: Test with Rat Embryo cells;
Result: positive
Source: Bayer AG Leverkusen
26-DEC-2001 (36)

5.8 Toxicity to Reproduction

Type: other
Species: rat Sex: male/female
Strain: Fischer 344
Route of admin.: oral feed
Exposure Period: 78 weeks
Frequency of treatment: continuous
Duration of test: 105 weeks
Doses: 0, 6.700, 12.100 mg/kg bw
Control Group: yes, concurrent no treatment
NOAEL Parental: > 12100 ppm
Method: other: EPA OTS 798.3300
Year: GLP: no data
Test substance: other TS: 1H-benzotriazole; purity > 99%
Remark: The 78 week oral study of 1H-benzotriazole in Fischer 344 rats did not find any evidence of dose-related pathology in the reproductive organs: prostate/testis/epididymis of males and uterus/ovaries of females. Findings, not significantly different from controls, included acute inflammation of the prostate, hyperplasia of the testis, acute inflammation, hydrometra, and hyperplasia of the uterus, inflammation and cyst formation of the ovaries.
Reliability: (2) valid with restrictions
Meets generally accepted scientific standards, well documented and acceptable for assessment
Flag: Critical study for SIDS endpoint
26-DEC-2001 (31)

Type: other
Species: mouse Sex: male/female
Strain: B6C3F1
Route of admin.: oral feed
Exposure Period: 104 weeks
Frequency of treatment: continuous
Duration of test: 106 weeks
Doses: 0, 11700, 23500 ppm
Control Group: yes, concurrent no treatment
NOAEL Parental: > 23500 ppm
Method: other: EPA OTS 798.3300
Year: GLP: no data
Test substance: other TS: 1H-benzotriazole; purity > 99%
Remark: The 104 week oral study of 1H-benzotriazole in mice did not find any evidence of pathology in the reproductive organs: prostate/testis/epididymis of males and uterus/ovaries of females. Findings, not significantly different from controls, included hyperplasia of the testis, hydrometra and cystic hyperplasia of the uterus, and cyst formation of the ovaries.
Reliability: (2) valid with restrictions
Meets generally accepted scientific standards, well documented and acceptable for assessment
Flag: Critical study for SIDS endpoint

5. Toxicity

Date: 26-DEC-2001

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26-DEC-2001

(31)

5.9 Developmental Toxicity/Teratogenicity

-

5.10 Other Relevant Information

Type: other

Remark: Extremely strong reaktion at nearly 160 degree C

Source: Bayer AG Leverkusen

28-JAN-1994

5.11 Experience with Human Exposure

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7. Risk Assessment

7.1 End Point Summary

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7.2 Hazard Summary

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7.3 Risk Assessment

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I U C L I D

D a t a S e t

Existing Chemical	ID: 29385-43-1
CAS No.	29385-43-1
EINECS Name	methyl-1H-benzotriazole
EINECS No.	249-596-6
Molecular Weight	133.2
Molecular Formula	C7H7N3

Producer Related Part

Company:
Creation date: 28-MAR-2000

Substance Related Part

Company:
Creation date: 28-MAR-2000

Memo: SOCMA, Benzotriazoles Coalition

Printing date: 05-DEC-2001
Revision date:
Date of last Update: 05-DEC-2001

Number of Pages: 31

Chapter (profile): Chapter: 1, 2, 3, 4, 5, 7
Reliability (profile): Reliability: without reliability, 1, 2, 3, 4
Flags (profile): Flags: without flag, confidential, non confidential, WGK (DE), TA-Luft (DE), Material Safety Dataset, Risk Assessment, Directive 67/548/EEC, SIDS

1. General Information

1.0.1 OECD and Company Information

Type: lead organisation
Name: Synthetic Organic Chemical Manufacturers Association (SOCMA),
Benzotriazoles Coalition
Street: 1850 M Street N.W., Suite 700
Town: 20036 Washington, D.C.
Country: United States
Phone: (202) 721-4100
Telefax: (202) 296-8120

05-DEC-2001

Type: cooperating company
Name: Bayer Corporation
Country: United States

05-DEC-2001

Type: cooperating company
Name: PMC Specialties Group, Inc.
Country: United States

05-DEC-2001

1.0.2 Location of Production Site

-

1.0.3 Identity of Recipients

-

1.1 General Substance Information

Substance type: organic
Physical status: solid
Purity: > 98 % w/w
05-DEC-2001

1.1.0 Details on Template

-

1.1.1 Spectra

-

1.2 Synonyms

Cobratec TT 100
05-DEC-2001

1. General Information

Methylbenzotriazole
05-DEC-2001

Preventol CI 7-100
05-DEC-2001

Tolyl triazole
05-DEC-2001

1.3 Impurities

-

1.4 Additives

-

1.5 Quantity

-

1.6.1 Labelling

-

1.6.2 Classification

-

1.7 Use Pattern

-

1.7.1 Technology Production/Use

-

1.8 Occupational Exposure Limit Values

-

1.9 Source of Exposure

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1.10.1 Recommendations/Precautionary Measures

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1.10.2 Emergency Measures

-

1. General Information

1.11 Packaging

-

1.12 Possib. of Rendering Subst. Harmless

-

1.13 Statements Concerning Waste

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1.14.1 Water Pollution

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1.14.2 Major Accident Hazards

-

1.14.3 Air Pollution

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1.15 Additional Remarks

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1.16 Last Literature Search

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1.17 Reviews

-

1.18 Listings e.g. Chemical Inventories

-

2. Physico-chemical Data

2.1 Melting Point

Value: 76 - 87 degree C
Method: other: Data from Handbook or collection of data
GLP: no data
Testsubstance: other TS: methyl-1H-benzotriazole; purity not noted
Reliability: (2) valid with restrictions
Data from Handbook or collection of data
Flag: Critical study for SIDS endpoint
05-DEC-2001 (1)

Value: 82 - 88 degree C
Testsubstance: as prescribed by 1.1 - 1.4
05-DEC-2001 (2)

2.2 Boiling Point

Value: 160 degree C at 2.67 hPa
Method: other: Data from Handbook or collection of data
GLP: no data
Testsubstance: other TS: methyl-1H-benzotriazole; purity not noted
Reliability: (2) valid with restrictions
Flag: Critical study for SIDS endpoint
05-DEC-2001 (1)

Value: > 200 degree C
Testsubstance: as prescribed by 1.1 - 1.4
05-DEC-2001 (2)

Value: > 300 degree C
Testsubstance: other TS: methyl-1H-benzotriazole; purity >99%
05-DEC-2001 (3)

2.3 Density

Type: density
Value: 1.13 g/cm3 at 100 degree C
Testsubstance: as prescribed by 1.1 - 1.4
Flag: Critical study for SIDS endpoint
05-DEC-2001 (2)

Type: bulk density
Value: 550 kg/m3
Testsubstance: as prescribed by 1.1 - 1.4
05-DEC-2001 (4)

2.3.1 Granulometry

-

2. Physico-chemical Data

2.4 Vapour Pressure

Value: .04 hPa at 50 degree C
Method: other (measured): Data from Handbook or collection of data
GLP: no data
Testsubstance: other TS: methyl-1H-benzotriazole; purity not noted
Reliability: (2) valid with restrictions
Data from Handbook or collection of data
Flag: Critical study for SIDS endpoint
05-DEC-2001 (1)

Value: .000277 hPa at 25 degree C
Method: other (calculated): MPBPWIN (v1.31)
Year: 1999
GLP: no
Testsubstance: other TS: molecular structure
Result: Vapor Pressure Estimations (25 deg C):
(Using BP: 311.65 deg C (estimated))
(Using MP: 97.46 deg C (estimated))
VP: 0.000147 mm Hg (Antoine Method)
VP: 0.000208 mm Hg (Modified Grain Method)
VP: 0.000385 mm Hg (Mackay Method)
Selected VP: 0.000208 mm Hg (Modified Grain Method)
Reliability: (2) valid with restrictions
Accepted calculation method
Flag: Critical study for SIDS endpoint
05-DEC-2001 (5)

Value: .00001 hPa at 25 degree C
GLP: no data
Testsubstance: as prescribed by 1.1 - 1.4
05-DEC-2001 (2)

Value: .04 hPa at 20 degree C
Testsubstance: other TS: methyl-1H-benzotriazole; purity >99%
Remark: estimated at 0.3 mmHg
05-DEC-2001 (3)

2.5 Partition Coefficient

log Pow: 1.71 at 25 degree C
Method: other (calculated): KOWWIN v1.65
Year: 1999
GLP: no
Testsubstance: other TS: molecular structure
Result: Log Kow(version 1.65
estimate): 1.71

SMILES : Cc1cccc2c1nnn2
CHEM : 1H-Benzotriazole, 4(or 5)-methyl-
MOL FOR: C7 H7 N3
MOL WT : 133.15

TYPE	NUM	LOGKOW	FRAGMENT DESCRIPTION	COEFF	VALUE
------	-----	--------	----------------------	-------	-------

Frag	1	-CH3 [aliphatic carbon]	0.5473	0.5473
Frag	6	Arom. Carbon	0.2940	1.7640
Frag	3	Arom. Nitrogen [5-member ring]	-0.5262	-1.5786
Factor	1	1,2,3-Triazole correction	0.7525	0.7525
Const		Equation Constant		0.2290

log Pow:	2.1
Method:	other (calculated)
Year:	
GLP:	no data
Testsubstance:	as prescribed by 1.1 - 1.4
05-DEC-2001	(6)

2.6.1 Water Solubility

Value: < .1 g/l at 18 degree C
Method: other: Data from Handbook or collection of data
GLP: no data
Testsubstance: other TS: methyl-1H-benzotriazole; purity not noted
Reliability: (2) valid with restrictions
Data from Handbook or collection of data
Flag: Critical study for SIDS endpoint
05-DEC-2001 (1)

Value: 5 g/l at 20 degree C
 Testsubstance: as prescribed by 1.1 - 1.4
 05-DEC-2001 (2)

Value: .55 vol% at 20 degree C
 Testsubstance: other TS: methyl-1H-benzotriazole; purity >99%
 05-DEC-2001 (3)

2.6.2 Surface Tension

2. Physico-chemical Data

2.7 Flash Point

Value: 180 degree C
Type:
Method: other: DIN 51376
Year:
GLP: no data
Testsubstance: as prescribed by 1.1 - 1.4
Reliability: (1) valid without restriction
Meets National standards method (AFNOR/DIN)

05-DEC-2001

(4)

2.8 Auto Flammability

-

2.9 Flammability

-

2.10 Explosive Properties

-

2.11 Oxidizing Properties

-

2.12 Additional Remarks

-

3. Environmental Fate and Pathways

3.1.1 Photodegradation

Type: air
INDIRECT PHOTOLYSIS
Sensitizer: OH
Conc. of sens.: 1560000 molecule/cm3
Rate constant: .000000000002746 cm3/(molecule * sec)
Degradation: 50 % after 3.9 day
Method: other (calculated): AOP Program (v1.89)
Year: 1999 GLP: no
Test substance: other TS: molecular structure
Reliability: (2) valid with restrictions
Accepted calculation method
Flag: Critical study for SIDS endpoint
05-DEC-2001

(5)

3.1.2 Stability in Water

-

3.1.3 Stability in Soil

-

3.2 Monitoring Data (Environment)

-

3.3.1 Transport between Environmental Compartments

Type: fugacity model level III
Media: other: air - sediment(s) - soil - water
Air (Level I):
Water (Level I):
Soil (Level I):
Biota (L.II/III):
Soil (L.II/III):
Method: other: EPIWIN Level III Fugacity Model
Year: 1999
Result:

Media Distribution (percent)	Half-Life (hr)	Emissions (kg/hr)	Fugacity (atm)
Air 2.77	93.5	1000	5.55e-011
Water 39.3	360	1000	2.61e-012
Soil 57.8	360	1000	5.31e-011
Sediment 0.0934	1.44e+003	0	2.06e-012

Media	Reaction (kg/hr)	Advection (kg/hr)	Reaction (percent)	Advection (percent)
Air	224	303	7.48	10.1
Water	827	429	27.6	14.3
Soil	1.22e+003	0	40.5	0
Sediment	0.491	0.0204	0.0164	0.000681

Persistence Time: 364 hr

3. Environmental Fate and Pathways

Reaction Time: 482 hr
Advection Time: 1.49e+003 hr
Percent Reacted: 75.6
Percent Advected: 24.4
Reliability: (2) valid with restrictions
Accepted calculation method
Flag: Critical study for SIDS endpoint
05-DEC-2001 (5)

3.3.2 Distribution

-

3.4 Mode of Degradation in Actual Use

-

3.5 Biodegradation

Type: aerobic
Inoculum: activated sludge, industrial
Concentration: 2 mg/l related to Test substance
Degradation: 77 % after 28 day
Method: OECD Guide-line 301 D "Ready Biodegradability: Closed Bottle Test"
Year: 1988 GLP: no
Test substance: as prescribed by 1.1 - 1.4
Remark: test conc.: 2.4, 8, 24, 80 mg/l
Reliability: (1) valid without restriction
Guideline study
Flag: Critical study for SIDS endpoint
05-DEC-2001 (6)

Type: aerobic
Inoculum: activated sludge
Concentration: 100 mg/l related to Test substance
Degradation: 4 % after 28 day
Method: other: "Manometric Respiration Test acc. to Directive 79/831/EEC, Annex V, Part C (July 1990)
Year: 1992 GLP: yes
Test substance: other TS: purity 99.9 %
Remark: inoculum adapted for 33d
Reliability: (1) valid without restriction
GLP Guideline study
Flag: Critical study for SIDS endpoint
05-DEC-2001 (6)

3.6 BOD5, COD or BOD5/COD Ratio

Method: other: Microbial Inhibition Test

Method: A series of test chambers containing a readily degradable primary substrate (d-glucose), dilution water, and inoculum were dosed with increasing amounts of Cobratec TT-100 (1 to 150 mg/l). Dilution water and primary substrate controls were conducted concurrently. The Dissolved Oxygen (DO) within each test chamber was measured after the addition of the test sample. The chambers were incubated in the dark for 3 days at a temperature of 18.9 to 20.6 degree C. The DO within each chamber was measured again after the incubation period.

Result: Inhibition of oxygen was not detected over the range of concentrations tested.

Test substance: other TS: tolyltriazole - Cobratec TT-100; purity not noted
05-DEC-2001 (7)

Method: other: Standard Biological Oxygen Demand Ttest (BOD)

Result: Concentrations as high as 2 mg/l will not exert any effect on a wastewater treatment facility.

Test substance: tolyltriazole; purity not noted
14-MAY-2001 (8)

Remark: ThOD: 1562 mg/g
Source: Bayer AG Leverkusen
06-SEP-1995

3.7 Bioaccumulation

-

3.8 Additional Remarks

-

4. Ecotoxicity

AQUATIC ORGANISMS

4.1 Acute/Prolonged Toxicity to Fish

Type: static
Species: Brachydanio rerio (Fish, fresh water)
Exposure period: 96 hour(s)
Unit: mg/l Analytical monitoring: no
LC0: 42
LC50: 65
Method: other: "Letale Wirkung beim Zebrabaerbling - Brachydanio rerio" (LC 0, LC 50, LC 100; 48-96 Stunden)
Verfahrensvorschlag Umweltbundesamt (Stand: Mai 1984)
Year: 1984 GLP: no
Test substance: as prescribed by 1.1 - 1.4
Reliability: (1) valid without restriction
Meets National standards method (AFNOR/DIN)
Flag: Critical study for SIDS endpoint
05-DEC-2001 (9)

Type: static
Species: Lepomis macrochirus (Fish, fresh water)
Exposure period: 96 hour(s)
Unit: mg/l Analytical monitoring: no data
LC50: 31
Method: other: according to Protocol issued by Pesticide Regulation
Division of EPA - January 20, 1971
Year: 1971 GLP: no data
Test substance: other TS: tolyltriazole - Cobratec TT-100; purity >99%
Result: Concentration Mortality
25.1 ppm 1/20
28.2 ppm 2/20
31.6 ppm 10/20
35.5 ppm 20/20
The LC50 is determined to be 31 ppm with 95% confidence limits
of 29.8 to 32.3 ppm.
Reliability: (1) valid without restriction
Meets National standards method (AFNOR/DIN)
Flag: Critical study for SIDS endpoint
05-DEC-2001 (10)

4. Ecotoxicity

Date: 05-DEC-2001
ID: 29385-43-1

Type:
Species: Pimephales promelas (Fish, fresh water)
Exposure period: 96 hour(s)
Unit: mg/l Analytical monitoring: no data
LC50: 25.5
Method: other: according to Protocol issued by Pesticide Regulation
Division of EPA - January 20, 1971
Year: 1971 GLP: no data
Test substance: other TS: tolyltriazole - Cobratec TT-100; purity >99%
Result: 96 hr 48 hr 24 hr
LC1 = 14.20 ppm 14.00 ppm 23.00 ppm
LC50 = 25.50 ppm 29.80 ppm 36.90 ppm
LC99 = 46.00 ppm 62.50 ppm 68.50 ppm
Reliability: (1) valid without restriction
Meets National standards method (AFNOR/DIN)
Flag: Critical study for SIDS endpoint
05-DEC-2001 (11)

Type:
Species: Salmo gairdneri (Fish, estuary, fresh water)
Exposure period: 96 hour(s)
Unit: mg/l Analytical monitoring: no data
LC50: 21.4
Method: other: according to Protocol issued by Pesticide Regulation
Division of EPA - January 20, 1971
Year: 1971 GLP: no data
Test substance: other TS: tolyltriazole - Cobratec TT-100; purity >99%
Result: 96 hr 48 hr
LC1 = 9.10 ppm 9.40 ppm
LC50 = 21.40 ppm 38.00 ppm
LC99 = 51.00 ppm *
Reliability: (1) valid without restriction
Meets National standards method (AFNOR/DIN)
Flag: Critical study for SIDS endpoint
05-DEC-2001 (12)

4. Ecotoxicity

4.2 Acute Toxicity to Aquatic Invertebrates

Type:
Species: Daphnia magna (Crustacea)
Exposure period: 48 hour(s)
Unit: mg/l Analytical monitoring:
EC0: 16
EC100: 78.4
geom. mean : 35.4
Method: other: Directive 67/548/EEC, (C.2) "Acute Toxicity for Daphnia" (29.12.1992)
Year: 1994 GLP: no
Test substance: other TS: methyl-1H-benzotriazole; purity 99.9 %
Remark: analyt. monit.: TOC
Source: Bayer AG Leverkusen
Reliability: (2) valid with restrictions
Flag: Critical study for SIDS endpoint
05-DEC-2001

Type:
Species: Daphnia magna (Crustacea)
Exposure period: 48 hour(s)
Unit: mg/l Analytical monitoring:
LC50 : 73.7
Method:
Year: GLP:
Test substance: other TS: methyl-1H-benzotriazole; purity >99%
05-DEC-2001

(3)

4.3 Toxicity to Aquatic Plants e.g. Algae

Species: Scenedesmus subspicatus (Algae)
Endpoint: growth rate
Exposure period: 72 hour(s)
Unit: mg/l Analytical monitoring:
EC50: 62
Method: other: "Algal Inhibition Test" (c.3), Directive 67/548/EEC (29.12.92)
Year: 1992 GLP: yes
Test substance: other TS: methyl-1H-benzotriazole; purity 99.9 %
Remark: Arithm. mean of analytically determined values:
Biomass
EC10: 10 mg/l
EC50: 32 mg/l
Growth rate
EC10: 24 mg/l
EC50: 62 mg/l
Dunnett-Test
NOEC: 7.5 mg/l
LOEC: 10.0 mg/l
Prior to the test, the TS was crushed with a pistil, weighed into water and treated in an ultrasonic bath for 30 minutes. All test results are related to TOC; 1 mg/l TOC equals 1.6 mg/l TS.

4. Ecotoxicity

Date: 05-DEC-2001
ID: 29385-43-1

Reliability: (1) valid without restriction
GLP Guideline study
Flag: Critical study for SIDS endpoint
05-DEC-2001 (13)

4.4 Toxicity to Microorganisms e.g. Bacteria

Type: aquatic
Species: activated sludge
Exposure period: 3 hour(s)
Unit: mg/l Analytical monitoring: no
EC50: 330
Method: other: E 3002: The Assessment of the Possible Inhibitory
Effect of Dyestuffs on Aerobic Waste Water Bacteria.
Experience with a Screening Test. Brown, D.; Hitz, H.R.;
Schaefer, L.: Chemosphere 10 (3), 245-261 (1981)
Year: 1982 GLP: no
Test substance:
05-DEC-2001 (6)

Type: aquatic
Species: Pseudomonas putida (Bacteria)
Exposure period: 30 minute(s)
Unit: mg/l Analytical monitoring: no
EC0: 31.25
Method: other: Bewertung toxischer Wasserinhaltsstoffe aus ihrer
Inhibitorwirkung auf die Substratoxydation von Pseudomonas
Stamm Berlin mit Hilfe polarographischer Sauerstoffmessungen.
Robra, K.H.: gwf wasser/abwasser 117 (2), 80-86 (1976)
Year: 1982 GLP: no
Test substance:
05-DEC-2001 (6)

4. Ecotoxicity

4.5 Chronic Toxicity to Aquatic Organisms

4.5.1 Chronic Toxicity to Fish

-

4.5.2 Chronic Toxicity to Aquatic Invertebrates

Species: Daphnia magna (Crustacea)
Endpoint:
Exposure period: 21 day
Unit: mg/l Analytical monitoring:
Method: OECD Guide-line 202, part 2 "Daphnia sp., Reproduction Test"
Year: 1995 GLP: yes
Test substance: other TS: methyl-1H-benzotriazole; purity 99.9 %
Remark: Arithm. mean of analytically determined values:
EC50 (Immobilisation): > 37.6 mg/l TS
> 23.5 mg/l TOC
EC50 (Reproduction): > 18.4 < 37.6 mg/l TS
> 11.5 < 23.5 mg/l TOC
NOEC (Reproduction): 18.4 mg/l TS
11.5 mg/l TOC
LOEC (Reproduction): 37.6 mg/l TS
23.5 mg/l TOC
Before starting the test, the TS was crushed with a pistil.
To produce the stock solution, the TS was weighed into
water, treated in an ultrasonic bath for 1 hour and
subsequently stirred on a magnetic stirrer for 24 hours.
Reliability: (1) valid without restriction
GLP Guideline study

05-DEC-2001

(6)

TERRESTRIAL ORGANISMS

4.6.1 Toxicity to Soil Dwelling Organisms

-

4.6.2 Toxicity to Terrestrial Plants

-

4.6.3 Toxicity to other Non-Mamm. Terrestrial Species

-

4.7 Biological Effects Monitoring

-

4.8 Biotransformation and Kinetics

-

4. Ecotoxicity

Date: 05-DEC-2001

ID: 29385-43-1

4.9 Additional Remarks

-

5. Toxicity

5.1 Acute Toxicity

5.1.1 Acute Oral Toxicity

Type: LD50
Species: rat
Strain:
Sex: male
Number of Animals: 5
Vehicle: other: corn oil
Value: 1470
Method:
Year: GLP: no data
Test substance: other TS: methylbenzotriazole; purity >99%
Method: The test substance was administered orally by stomach tube to six groups of 5 male albino rats (weight range 247 - 345 g). The sample was administered in corn oil as a 10% or 50% wt/vol suspension. (Dosage levels of 46.4, 100, 215 mg/kg as 10 % wt/vol; 464, 1000, 2150 mg/kg as 50% wt/vol).

Food was withheld for 18 hrs prior to dosing, following which food and water was supplied ad libitum. All animals were observed several times during day of dosing for gross signs of systemic toxicity and mortality and daily thereafter for 14 days. Gross autopsies were done on all animals. Statistical analysis of mortality data was done by "moving average" method (Weil, CS. Biometrics. 8:249. 1952).

Result: LD 50 = 1470 mg/kg bw (95% conf. limit could not be calculated due to "all or none" response.)

Time of death	Dose (mg/kg)					
	46.4	100	215	464	1000	2150
1 hr	0/5	0/5	0/5	0/5	0/5	0/5
2 hr	0/5	0/5	0/5	0/5	0/5	0/5
4 hr	0/5	0/5	0/5	0/5	0/5	0/5
24 hr	0/5	0/5	0/5	0/5	0/5	5/5
2 days	0/5	0/5	0/5	0/5	0/5	5/5
3 days	0/5	0/5	0/5	0/5	0/5	5/5
4 days	0/5	0/5	0/5	0/5	0/5	5/5
5 days	0/5	0/5	0/5	0/5	0/5	5/5
6 days	0/5	0/5	0/5	0/5	0/5	5/5
7-14 days	0/5	0/5	0/5	0/5	0/5	5/5

Reliability: (2) valid with restrictions
Meets generally accepted scientific standards, well documented and acceptable for assessment
Flag: Critical study for SIDS endpoint

05-DEC-2001

(14)

5. Toxicity

Type: LD50
Species: rat
Strain: other: FDRL strain
Sex: male/female
Number of Animals: 5
Vehicle: CMC
Value: 1830 mg/kg bw
Method: other: as recommended in "Appraisal of Safety of Chemicals in Food, Drugs, and Cosmetics" Association of Food and Drug Officials of the US. 1959
Year: 1959 GLP: no data
Test substance: other TS: tolutriazole, OLIN 58734; purity not noted
Result: LD 50 = 1830 mg/kg bw (95% conf. limit = 1200-2810 mg/kg)

MORTALITY DATA

Time of death	Dose (mg/kg)				
	500	1000	2000	4000	8000
5 min	0/5	0/5	0/5	5/5	5/5
1/2 -3 hr	0/5	0/5	3/5	5/5	5/5
7 days	1/5	0/5	3/5	5/5	5/5

Observations:

500 mg/kg - CNS depression, shallow breathing, nasal bleeding
1000 mg/kg - CNS depression
2000 mg/kg - CNS depression, shallow breathing
4000 mg/kg - CNS depression, shallow breathing, eyes tearing
8000 mg/kg - CNS depression, salivation

Reliability: (2) valid with restrictions
Meets generally accepted scientific standards, well documented and acceptable for assessment
Flag: Critical study for SIDS endpoint
05-DEC-2001 (15)

Type: LD50
Species: rat
Strain:
Sex: male/female
Number of Animals: 10
Vehicle:
Value: 1625 ml/kg bw
Method: EPA OTS 798.1175
Year: GLP: no data
Test substance: other TS: tolyltriazone residue; purity not noted
Reliability: (2) valid with restrictions
Meets National standards method (AFNOR/DIN)
05-DEC-2001 (16)

5. Toxicity

Type: LD50
Species: rat
Strain:
Sex:
Number of
Animals:
Vehicle:
Value: 675
Method:
Year: GLP:
Test substance: other TS: tolyltriazole - Cobratec TT-100; purity >99%
05-DEC-2001 (17)

Type: LD50
Species: rat
Strain: Wistar
Sex: male/female
Number of
Animals: 10/dose
Vehicle: DMSO
Value: 720 mg/kg bw
Method:
Year: GLP: no data
Test substance: as prescribed by 1.1 - 1.4
05-DEC-2001 (6)

Type: LD50
Species: rat
Strain:
Sex:
Number of
Animals:
Vehicle:
Value: 675 mg/kg bw
Method:
Year: GLP:
Test substance: other TS: methyl-1H-benzotriazole; purity not noted
05-DEC-2001 (1) (3)

Type: LD50
Species: rat
Strain:
Sex:
Number of
Animals:
Vehicle:
Value: 1600 mg/kg bw
Method:
Year: GLP:
Test substance: other TS: methyl-1H-benzotriazole; purity not noted
05-DEC-2001 (1)

5. Toxicity

5.1.2 Acute Inhalation Toxicity

Type: other: Acute Inhalation Toxicity
Species: rat
Strain: Sprague-Dawley
Sex: male/female
Number of Animals: 20
Vehicle:
Exposure time: 1 hour(s)
Value: > 1.73 mg/l
Method:
Year: GLP: no data
Test substance: other TS: tolyltriazole; purity not noted
Method: Ten male and 10 female Sprague-Dawley rats were exposed for one hour to an aerosol of tolyltriazole at actual concentration of 1.73 +/- 0.67 mg/l, and EAD of 0.35 micron, a geometric standard deviation of 2.62 ug/l. The animals were observed for toxicity and mortality during the exposure and daily for a 14 day post-exposure period. All animals were necropsied and all organs observed for gross abnormalities.
Result: No deaths occurred during the 14 day post-exposure period. No significant pharmacologic or toxicologic signs were noted. All animals appeared in good health post-exposure and gained weight normally. The primary effect observed on necropsy was pulmonary irritation.
Reliability: (2) valid with restrictions
Meets generally accepted scientific standards, well documented and acceptable for assessment
Flag: Critical study for SIDS endpoint
05-DEC-2001 (18)

5.1.3 Acute Dermal Toxicity

Type: LD50
Species: rabbit
Strain:
Sex: male/female
Number of Animals: 4
Vehicle: water
Value: > 4000 mg/kg bw
Method: other: as recommended in "Appraisal of Safety of Chemicals in Food, Drugs, and Cosmetics" Association of Food and Drug Officials of the US. 1959
Year: 1959 GLP: no data
Test substance: other TS: tolutriazole, OLIN 58734; purity not noted
Result: No deaths occurred at any dose level in 14 days. No noteworthy findings were observed.

Primary irritation scores -
500 mg/kg = 1.4
1000 mg/kg = 1.5

5. Toxicity

2000 mg/kg = 1.1
4000 mg/kg = 1.4
Reliability: (2) valid with restrictions
Meets generally accepted scientific standards, well documented
and acceptable for assessment
Flag: Critical study for SIDS endpoint
05-DEC-2001 (15)

Type: LD50
Species: rabbit
Strain:
Sex:
Number of
Animals: 10
Vehicle:
Value: > 2000 mg/kg bw
Method: other: Huntingdon Reserach Center protocol
Year: GLP: no data
Test substance: other TS: Cobratec TT-100 (tolyltriazole); purity not noted
Reliability: (2) valid with restrictions
Meets generally accepted scientific standards, well documented
and acceptable for assessment
Flag: Critical study for SIDS endpoint
05-DEC-2001 (19)

5.1.4 Acute Toxicity, other Routes

Type: LD50
Species: rat
Strain:
Sex:
Number of
Animals:
Vehicle:
Route of admin.: i.p.
Value:
Method:
Year: GLP:
Test substance:
Remark: male: 172 mg/kg
female: 237 mg/kg
05-DEC-2001 (6)

5. Toxicity

5.2 Corrosiveness and Irritation

5.2.1 Skin Irritation

Species: rabbit
Concentration:

Exposure:
Exposure Time:
Number of
Animals:

PDII:
Result: not irritating

EC classificat.:

Method:

Year: GLP:

Test substance:

Remark: exposure time: 4 hours

05-DEC-2001

(6)

5.2.2 Eye Irritation

Species: rabbit
Concentration: undiluted
Dose: 10 other: mg

Exposure Time:

Comment: not rinsed

Number of
Animals:

Result: slightly irritating

EC classificat.:

Method: other: as recommended in "Appraisal of Safety of Chemicals in Food, Drugs, and Cosmetics" Association of Food and Drug Officials of the US. 1959. p. 46

Year: 1959 GLP: no data

Test substance: other TS: tolutriazole, OLIN 58734; purity not noted

Result: Irritation Score:

Rabbit No. & sex	day 1	day 2	day 3
2201M	6	2	0
2202M	23	2	0
2203M	45	24	24
2204F	4	0	0
2205F	20	12	2
2206F	10	4	0

(maximum irritation score = 110)

Reliability: (1) valid without restriction

Meets generally accepted scientific standards, well documented and acceptable for assessment

05-DEC-2001

(15)

5. Toxicity

Species: rabbit
Concentration:
Dose:
Exposure Time:
Comment:
Number of
Animals:
Result: not irritating
EC classificat.:
Method:
Year: GLP:
Test substance:
05-DEC-2001 (6)

5.3 Sensitization

Type: Guinea pig maximization test
Species: guinea pig
Number of
Animals:
Vehicle:
Result: not sensitizing
Classification:
Method:
Year: GLP:
Test substance:
05-DEC-2001 (6)

5.4 Repeated Dose Toxicity

Species: rat Sex:
Strain: Wistar
Route of admin.: gavage
Exposure period: 29 d
Frequency of
treatment: daily
Post. obs.
period:
Doses: 0, 50, 150, 450 mg/kg
Control Group: yes, concurrent vehicle
NOAEL: 150 mg/kg
Method:
Year: GLP:
Test substance: as prescribed by 1.1 - 1.4
Result: In the highest dose group signs of mild apathy could be
observed. Haematological and histopathological results were
within the reference ranges.
Reliability: (2) valid with restrictions
Meets generally accepted scientific standards, well documented
and acceptable for assessment
Flag: Critical study for SIDS endpoint
05-DEC-2001 (20)

5. Toxicity

Date: 05-DEC-2001
ID: 29385-43-1

Species: rat Sex:
Strain:
Route of admin.: gavage
Exposure period: 9 d
Frequency of treatment: 1/d
Post. obs. period:
Doses: 0, 100, 500 mg/kg
Control Group:
Method:
Year: GLP:
Test substance:
Remark: Lethargy and respiratory difficulties after each dose; no macroscopic noticeable changes to organs and tissues. [Sedation und Atembeschwerden nach jeder Applikation der naechsten Dosis; krinr makroskopischen Auffaelligkeiten an Organen und Geweben]
Source: Bayer AG Leverkusen
05-DEC-2001 (6)

5.5 Genetic Toxicity 'in Vitro'

Type: Ames test
System of testing: Salmonella typhimurium TA-1535, 1537, 1538, 98, 100
Concentration: 0.80, 0.4, 2, 10 mg/plate
Cytotoxic Conc.: 10 mg/ plate
Metabolic activation: with and without
Result: negative
Method: EPA OTS 798.5265
Year: GLP: no data
Test substance: other TS: Cobratec TT-100 (tolyltriazole); purity >99%
Remark: Activation system liver homogenate was prepared from Sprague-Dawley adult male rats induced by Arochlor 1254, five days before sacrifice.
Result: The revertant response elicited at the highest concentration indicated a slight elevation of the revertant rate but did not produce a response of at least 2x background and is negated by the toxicity of the compound.
Reliability: (1) valid without restriction
Meets National standards method (AFNOR/DIN)
Flag: Critical study for SIDS endpoint
05-DEC-2001 (21)

5. Toxicity

Date: 05-DEC-2001
ID: 29385-43-1

Type: DNA damage and repair assay
 System of testing: Human embryonic lung fibroblasts (WI-38)
 Concentration: 0.8, 8, 40, 80 ug/plate
 Cytotoxic Conc.: EC50 = 20 ug/plate as determined by screening cytotoxicity assay
 Metabolic activation: without
 Result: negative
 Method: EPA OTS 798.5550
 Year: GLP: no data
 Test substance: other TS: Cobratec TT-100 (tolyltriazole); purity >99%
 Result: Cobratec TT-100 did not elicit significant 3H-TdR incorporations above control levels at any dose level tested.
 Reliability: (1) valid without restriction
 Meets National standards method (AFNOR/DIN)
 Flag: Critical study for SIDS endpoint
 05-DEC-2001 (21)

Type: other: Mouse fibroblast Transformation Assay
 System of testing: C3H 10T1/2 mouse embryonic fibroblastic cell line
 Concentration: 6, 60, 600 ug/plate
 Cytotoxic Conc.: EC50 = 4 ug/plate as determined by screening cytotoxicity assay
 Metabolic activation: without
 Result: negative
 Method:
 Year: GLP: no data
 Test substance: other TS: Cobratec TT-100 (tolyltriazole); purity not noted
 Method: Two sets of 60mm culture dishes are seeded with cells. One set of dishes, 12 replicates per dose, is seeded with 1000 cells. This set is used for the transformation assay. The second set was seeded with 200 cells per dish, 3 replicates/dose, and is utilized for cytotoxicity determinations.

Both sets of cells are treated in an identical manner with solutions of the test material. Following a 24-hour exposure period, the toxicant is washed from all plates and the cells refed with normal growth media. Ten days following the initial seeding, the plates designated for cytotoxicity assay are washed, fixed with methanol, and stained. The clones on all plates are counted and the plating efficiency counted. This plating efficiency is expressed as the number of colonies formed as a percentage of the number of cells seeded.

The transformation plates are incubated for 6 weeks with weekly medium changes. During this time, the clones grow to form a confluent monolayer of cells on the bottom of the plates. At the termination of the incubation period, all remaining plates are washed, fixed, stained and scored for transformed foci.

Type I foci : tightly packed cells
 Type II foci : massive piling into opaque multilayers
 Type III foci : highly polar, densely stained cells, which form a criss-crossed multilayer

Type II and III are considered to be malignantly transformed. The transformation frequency is calculated as the percentage of cells that give rise to transformed foci corrected for plating efficiency, which is determined by the cytotoxicity assay.

Remark: The C3H 10T1/2 line is a fibroblastic cell line, derived from C3H mouse embryos which are highly sensitive to postconfluence inhibition of cell division. When C3H 10T1/2 cells are exposed to a variety of chemical carcinogens, morphologically transformed foci develop with a frequency that is dose dependent. The foci have been shown to produce fibrosarcomas when injected into syngenic mice. Therefore, the C3H 10T1/2 cell line can be used to assay for chemical carcinogens.

Result: Cobratec TT-100 did not produce significant increases in transformation above control cell population levels. As a positive control, the cells did respond in a dose-dependent manner to the chemical carcinogen dimethylbenzanthracene (DMBA).

05-DEC-2001

(21)

Type: Ames test

System of testing: Salmonella typhimurium TA97, TA98, TA100, TA1535, TA1537

Concentration: 0, 33, 100, 333, 1000, 1666, 3333, 6666 ug/plate

Cytotoxic Conc.: strain TA1535 cytotoxic at 6666 ug/plate

Metabolic activation: with and without

Result:

Method:

Year: GLP: no data

Test substance: other TS: tolyltriazole, CAS#29385-43-1, obtained from Sherwin Williams; purity >99%

Remark: Solvent: DMSO

Metabolic activation: HLI= Aroclor-induced hamster liver S-9
 RLI=Aroclor-induced rat liver S-9

Result:

Strain	TA100	TA1535	TA97	TA98
NA	-	-	-	-
5% HLI	?	NT	NT	-
10% HLI	?	-	-	?
+w				
?				
30%HLI	-	NT	NT	-
5% RLI	+	NT	NT	NT
10% RLI	?	-	-	-
+				
?				
30% RLI	+w	NT	NT	NT

- = non-mutagenic
 ? = questionable mutagenic response

5. Toxicity

+w = weakly mutagenic
+ = mutagenic
NT = not-tested
05-DEC-2001 (22)

Type: Ames test
System of testing: Salmonella typhimurium
Concentration:
Cytotoxic Conc.:
Metabolic activation: with and without
Result: negative
Method:
Year: GLP:
Test substance:
Source: Bayer AG Leverkusen
05-DEC-2001 (6)

5.6 Genetic Toxicity 'in Vivo'

Type: Micronucleus assay
Species: mouse Sex: male/female
Strain: other: Bor. NMRI; manufacturer Winkelmann
Route of admin.: oral unspecified
Exposure period: single exposure
Doses: 600 mg/kg
Result: negative
Method: OECD Guide-line 474 "Genetic Toxicology: Micronucleus Test"
Year: 1987 GLP: yes
Test substance: other TS: Preventol CI 7-100; purity 99,3 %
Reliability: (1) valid without restriction
GLP Guideline study
Flag: Critical study for SIDS endpoint
05-DEC-2001 (23)

5.7 Carcinogenicity

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5.8 Toxicity to Reproduction

Remark: The 78 week oral study of 1H-benzotriazole (95-14-7) in Fischer 344 rats and the 104 week oral study of 1H-benzotriazole in B6C3F1 mice did not find any evidence of pathology in the reproductive organs. The organs examined were: prostate/testis/epididymis of males and uterus/ovaries of females.
06-DEC-2001 (24)

5. Toxicity

5.9 Developmental Toxicity/Teratogenicity

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5.10 Other Relevant Information

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5.11 Experience with Human Exposure

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6. References

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- (2) Safety Data Sheet Bayer AG, 15.06.2000
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7. Risk Assessment

7.1 End Point Summary

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7.2 Hazard Summary

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7.3 Risk Assessment

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